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A Study of Rosenbrock-Type Methods of High Order

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Summary. This paper deals with the solution of nonlinear stiff ordinary differential equations. The methods derived here are of Rosenbrock-type. This has the advantage that they are A-stable (or stiffly stable) and nevertheless do not require the solution of nonlinear systems of equations. We derive methods of orders 5 and 6 which require one evaluation of the Jacobian and one LU decomposition per step. We have written programs for these methods which use Richardson extrapolation for the step size control and give numerical results.

Subject Classifications: AMS(MOS): 65L05 CR: 5.17.

1. Definition of the Method

a) Formulation for an Autonomous System

We consider the numerical solution of the initial value problem

$$y'(x)=f(y(x)), \qquad y(x_0)=y_0 \tag{1}$$

defined on some real or complex space. Given a step size h we want to find an approximation y_1 to $y(x_0+h)$.

Let a_{ij}, c_{ij}, m_i $(i=1, \ldots, s, j=1, \ldots, i-1)$ and γ be given parameters. Then the corresponding Rosenbrock (or ROW) method is defined by

$$E=I-\gamma h f'(y_0), \tag{2a}$$

$$Ek_i=f\left(y_0+h\sum_{j=1}^{i-1} a_{ij}k_j\right)+\sum_{j=1}^{i-1} c_{ij}k_j \qquad (i=1, \ldots, s), \tag{2b}$$

$$y_1=y_0+h\sum_{i=1}^{s} m_i k_i. \tag{2c}$$

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In (2a) the computation of the Jacobian of the system is required. Formula (2b) consists in a sequence of s linear equations for the computation of the vectors k_i. All these equations have the same matrix E, so that only one LU factorization is necessary per step.

b) Formulation for Nonautonomous Systems

For

$$y'(x)=f(x, y(x)), \qquad y(x_0)=y_0 \tag{3}$$

the above method becomes

$$E=I-\gamma h f_y(x_0, y_0), \tag{4a}$$

$$Ek_i=f\left(x_0+A_i h, y_0+\sum_{j=1}^{i-1} a_{ij}k_j\right)+B_i h f_x(x_0, y_0)+\sum_{j=1}^{i-1} c_{ij}k_j, \quad (i=1, \dots, s) \tag{4b}$$

$$y_1=y_0+h\sum_{i=1}^{s} m_i k_i \tag{4c}$$

where

$$B_1=\gamma, \qquad B_i=\gamma+\sum_{j=1}^{i-1} c_{ij}B_j \ (i=2, s), \qquad A_i=\sum_{j=1}^{i-1} a_{ij}B_j/\gamma \ (i=1, s).$$

c) Formulation for Implicit Differential Equations

For

$$My'(x)=f(x, y(x)), \qquad y(x_0)=y_0$$

the method can be written as

$$E=M-\gamma h f_y(x_0, y_0),$$

$$Ek_i=f\left(x_0+A_i h, y_0+h\sum_{j=1}^{i-1} a_{ij}k_j\right)+B_i h f_x(x_0, y_0)+M\sum_{j=1}^{i-1} c_{ij}k_j,$$

$$y_1=y_0+h\sum_{i=1}^{s} m_i k_i.$$

This formulation is obtained by writing E for ME and avoids the inversion of M.

d) Equivalent Formulation with the Jacobian

Method (2) is also equivalent with

$$u_i=y_0+\sum_{j=1}^{i-1} \alpha_{ij}g_j \tag{5a}$$

$$g_i = hf(u_i) + hf'(y_0) \sum_{j=1}^{i} \gamma_{ij} g_j \qquad (i=1, s), \tag{5b}$$

$$y_1 = y_0 + \sum_{i=1}^{s} \mu_i g_i \tag{5c}$$

where the coefficients satisfy

$$\begin{aligned} c_{ij} &= \sum_{k=1}^{i-1} \gamma_{ik}(\delta_{kj} - c_{kj})/\gamma, \qquad a_{ij} = \sum_{k=1}^{i-1} \alpha_{ik}(\delta_{kj} - c_{kj}), \qquad \gamma_{ii} = \gamma, \\ m_j &= \sum_{k=1}^{s} \mu_k(\delta_{kj} - c_{kj}). \qquad (i, j = 1, s). \end{aligned} \tag{5d}$$

This can be seen by using $I = E + \gamma h f'(y_0)$, by putting $g_i = h\left(k_i - \sum_{j=1}^{i-1} c_{ij} k_j\right)$, and by some formula manipulation. This formulation is the classical one (see e.g. Nørsett-Wolfbrandt [5]), but less adapted to numerical computations. We shall use it below to derive the order conditions.

Remarks. Similar methods of orders 3 and 4 have first been proposed by Rosenbrock [1], Calahan [2], van der Houwen [3], Wolfbrandt [4], Nørsett-Wolfbrandt [5], Kaps-Rentrop [6] and [13, 14]. Much work is published on methods with $c_{ij} = 0$, named "semi-implicit RK methods", see e.g. [15].

2. Derivation of Order Conditions

For the order conditions we have to study the power series in h of y_1, g_i, and u_i defined in (5). These turn out to be "Butcher series"

$$B(\mathbf{a}, y_0) = \sum_{t \in LT} \frac{h^{\rho(t)}}{\rho(t)!} \mathbf{a}(t) F(t)(y_0)$$

as defined in [7-9]. We are thus using the notation of these papers. In addition we call a node of a tree $t \in LT$ *singly-branched* if exactly one upward branch leaves this node. In the Definition 2 of [9] this means that for this node $\operatorname{card}(t^{-1}(i)) = 1$.

1. Theorem. *The functions u_i, g_i, y_1 of* (5) *are Butcher series*

$$u_i(h) = B(\mathbf{u}_i, y_0), \qquad g_i(h) = B(\mathbf{g}_i, y_0), \qquad y_1(h) = B(\mathbf{y}_1, y_0)$$

whose coefficients $\mathbf{u}_i(t)$, $\mathbf{g}_i(t)$, $\mathbf{y}_1(t)$, $t \in T$ are recursively defined by

$$\mathbf{u}_i(\emptyset) = 1, \qquad \mathbf{u}_i(t) = \sum_{j=1}^{i-1} \alpha_{ij} \mathbf{g}_j(t) \qquad (t \neq \emptyset), \tag{6a}$$

$$\mathbf{g}_i(\emptyset) = 0, \qquad \mathbf{g}_i(\tau) = 1, \tag{6b}$$

$$\mathbf{g}_i(t)=\rho(t)\,\mathbf{u}_i(t_1)\dots\mathbf{u}_i(t_m)+\begin{cases}0 & \text{if } t=[t_1,\dots,t_m],\ m>1\\ \rho(t)\sum_{j=1}^{i}\gamma_{ij}\mathbf{g}_j(t_1) & \text{if } t=[t_1].\end{cases}$$

$$\mathbf{y}_1(\emptyset)=1,\qquad \mathbf{y}_1(t)=\sum_{i=1}^{s}\mu_i\mathbf{g}_i(t). \tag{6c}$$

Proof. (6a) and (6c) follow directly from (5a) and (5c). As proved in [8] (Theorem 13 or Theorem 6), $hf(u_i)=B(\mathbf{u}_i', y_0)$ is a Butcher series with coefficients $\mathbf{u}_i'(t)=\rho(t)\,\mathbf{u}_i(t_1)\dots\mathbf{u}_i(t_m)$. This yields the first term of (6b). As for the second term we see from $f'(y_0)\,F(t_1)(y_0)=F([t_1])(y_0)$ that

$$hf'(y_0)\,g_j(h)=\sum_{\substack{t\in LT\\ t=[t_1]}}\rho(t)\frac{h^{\rho(t)}}{\rho(t)!}\mathbf{g}_j(t_1)\,F(t)(y_0)$$

is a Butcher series whose only non-zero terms belong to trees with a singly-branched root. □

Remark. This last part of the proof is a special case of Theorem 2.2 of [5].

To simplify formulas (6), we put

$$\alpha_{ij}=0\ \ j\geqq i,\qquad \gamma_{ij}=0\ \ j>i,\qquad \beta_{ij}'=\alpha_{ij}+\gamma_{ij},\qquad \beta_{ij}=\begin{cases}\beta_{ij}' & i>j\\ 0 & i=j.\end{cases} \tag{7}$$

$$\Gamma(\tau)=1,\qquad \Gamma(t)=\rho(t)\,\Gamma(t_1)\dots\Gamma(t_m)\qquad \text{for } t=[t_1,\dots,t_m].$$

Then by inserting (6a) and (6b) into (6c) we obtain:

2. Theorem. *For every tree $t \neq \emptyset$ the coefficients of y_1 are given by*

$$\mathbf{y}_1(t)=\Gamma(t)\sum_{i=1}^{s}\mu_i\,\Psi_i(t) \tag{8}$$

where the $\Psi_i(t)$ are defined recursively

$$\Psi_i(\tau)=1$$

$$\Psi_i(t)=\begin{cases}\sum_{j_1,\dots,j_m}\alpha_{ij_1}\dots\alpha_{ij_m}\Psi_{j_1}(t_1)\dots\Psi_{j_m}(t_m) & \text{for } t=[t_1,\dots,t_m]\ m>1.\\ \sum_j\beta_{ij}'\Psi_j(t_1) & \text{for } t=[t_1].\ \ \square\end{cases} \tag{9}$$

The expressions $\Psi_i(t)$ which result from the recursion (9) can easily be obtained from the shape of the tree: One has to attach to each node of t a summation letter starting with "i" at the root. Then Ψ_i is the sum over a product consisting of

β_{jk}' – whenever a singly-branched node "j" is directly connected with an upper node "k";

α_{jk} – whenever a multiply-branched node "j" is directly connected with an upper node "k".

3. Example. For the tree sketched in Fig. 1 we have

$$\mathbf{y}_1(\mathrm{t})=7.2.3\sum_i\mu_i\Psi_i(t),\qquad \Psi_i(t)=\sum_{k,j,l,m,n,p}\alpha_{ik}\beta_{kl}'\alpha_{ij}\alpha_{jm}\alpha_{jn}\alpha_{ip}.$$

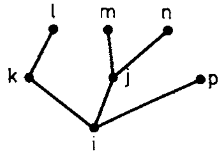


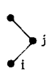
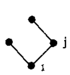
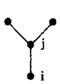
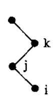
Fig. 1

In these expressions the summation over the maximal nodes (l, m, n, p in the above example) can be eliminated by introducing

$$\alpha_i = \sum_j \alpha_{ij}, \qquad \beta'_i = \sum_j \beta'_{ij}, \qquad \beta_i = \sum_j \beta_{ij}. \tag{10}$$

Then Example 3 becomes $\Psi_i(t) = \sum_{j,k} \alpha_{ik} \beta'_k \alpha_{ij} \alpha_j^2 \alpha_i$. Table 1 gives the resulting expressions for all trees with $\rho(t) \leqq 4$.

Table 1

Number	t	$\rho(t)$	$\Gamma(t)$	$\sum \mu_i \Psi_i$
1		1	1	$\sum \mu_i$
2		2	2	$\sum \mu_i \beta'_i$
3		3	3	$\sum \mu_i \alpha_i^2$
4		3	6	$\sum \mu_i \beta'_{ij} \beta'_j$
5		4	4	$\sum \mu_i \alpha_i^3$
6		4	8	$\sum \mu_i \alpha_i \alpha_{ij} \beta'_j$
7		4	12	$\sum \mu_i \beta'_{ij} \alpha_j^2$
8		4	24	$\sum \mu_i \beta'_{ij} \beta'_{jk} \beta'_k$

As the exact solution $y(x_0+h)$ of (1) is a Butcher series with coefficients $\mathbf{y}(t) = 1$ for all $t \in T$ (see [8], Example 3), we have

4. Corollary. *Method* (5) *is of order p iff*

$$\sum_i \mu_i \Psi_i(t) = 1/\Gamma(t) \qquad \text{if } \rho(t) \leqq p \tag{11}$$

and this equation is not true for at least one tree of order $p+1$.

The principal truncation error is then

$$\sum_{t \in LT,\, \rho(t) = p+1} \frac{h^{p+1}}{(p+1)!} (1 - \mathbf{y}_1(t))\, F(t)(y_0),$$

so that we call the expressions $\mathbf{e}(t)=1-\mathbf{y}(t)$ the *error coefficients* and $C=\max_{\rho(t)=p+1}(|\mathbf{e}(t)|/(p+1)!)$ the *error constant* (which sometimes differs with definitions of other papers by the factor $\alpha(t)$).

3. Simplification of the Order Conditions

The above conditions can be simplified by two procedures. Firstly

5. Theorem. *Let u_1, u_2, v_1, v_2, v_3 be trees as sketched in Fig. 2, where the encircled parts are assumed to be identical.*

a) *The condition*

$$\sum_k \alpha_{ik}\beta'_k=\alpha_i^2/2 \quad \text{or} \quad \sum_k \alpha_{ik}\beta_k=\alpha_i(\alpha_i/2-\gamma) \qquad (2\leqq i\leqq s) \tag{12}$$

implies that $\mathbf{y}_1(u_1)=\mathbf{y}_1(u_2)$.

b) *The condition*

$$\sum_i \mu_i\beta'_{ik}=\mu_k(1-\alpha_k) \quad \textit{or} \quad \sum_i \mu_k\beta_{ik}=\mu_k(1-\alpha_k-\gamma) \qquad (1\leqq k\leqq s) \tag{13}$$

implies that

$$\mathbf{y}_1(v_1)=1 \quad \textit{and} \quad \mathbf{y}_1(v_2)=1 \qquad \textit{imply} \;\; \mathbf{y}_1(v_3)=1. \;\; \square$$

The proof (direct verification) is omitted. Similar "simplifying assumptions" appear, since Butcher, throughout the literature on high-order methods.

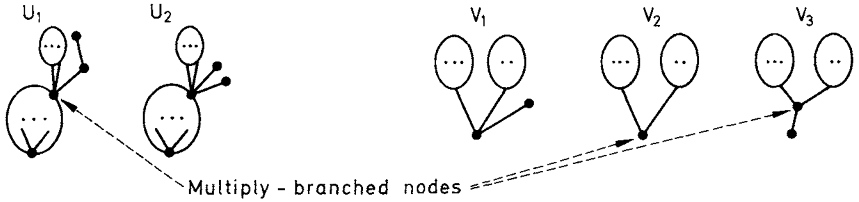


Fig. 2

Secondly we use $\beta'_{ii}=\gamma_{ii}=\gamma$ for all i and move all terms that contain γ to the right hand side of (11). This gives, using previous order conditions, a polynomial in γ and the number of terms in Ψ_i is considerably reduced. So we denote by $\Phi_i(t)$ the expressions which are defined in exactly the same way as Ψ_i in (9) with the exception that β'_{ij} is replaced by β_{ij}. Further, for $t\in T$ and j a positive integer we define

$$V(t,j)=\{s\in T;\ s \text{ appears from } t \text{ by removing } j \text{ singly-branched nodes}\}.$$

If t has less that j singly-branched nodes, then $V(t,j)=\emptyset$. If $s\in V(t,j)$, we denote

$$N(t,s)=\text{number of possibilities to obtain } s \text{ by removing } j \text{ singly-branched nodes from } t.$$

6. Theorem. *If the order conditions* (11) *are satisfied for all trees of order* $\leqq \rho(t)-1$, *then*

$$\sum_i \mu_i \Phi_i(t) = \sum_{j \geqq 0} (-\gamma)^j \sum_{s \in V(t,j)} N(t,s)/\Gamma(s) \tag{14}$$

is equivalent to (11) *for t.*

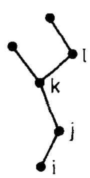
Proof. If we insert in $\Phi_i(t)$ $\beta_{ij} = (\beta'_{ij} - \gamma\delta_{ij})$ and multiply out the powers of γ, we obtain

$$\sum_i \mu_i \Phi_i(t) = \sum_{j \geqq 0} (-\gamma)^j \sum_{s \in V(t,j)} N(t,s) \sum_i \mu_i \Psi_i(s).$$

By hypothesis we now replace $\sum \mu_i \Psi_i(s)$ by $1/\Gamma(s)$ and obtain (14). □

7. *Example.* An example is presented in Fig. 3. Thus the corresponding order condition is

$$\sum_{i,j,k,l} \mu_i \beta_{ij} \beta_{jk} \alpha_k \alpha_{kl} \beta_l = \frac{1}{240} - \frac{\gamma}{15} + \frac{7\gamma^2}{24} - \frac{\gamma^3}{3}.$$



t

j	1	1	2	2	3
s					
N(t, s)	2	1	2	1	1
Γ(s)	5.4.2	5.4.3	4.3	4.2	3

Fig. 3

8. Table 2. Simplified order conditions for Order 6

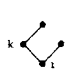
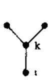
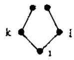
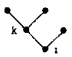
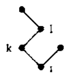
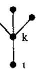
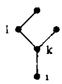
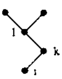
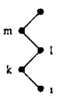
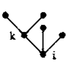
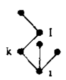
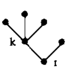
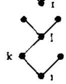
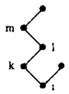
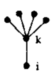
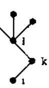
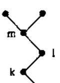
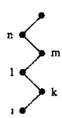
Number	Tree	$\rho(t)$	Condition
1		1	$\sum \mu_i = 1$
2		2	$\sum \mu_i \beta_i = \frac{1}{2} - \gamma = p_2$
3		3	$\sum \mu_i \alpha_i^2 = \frac{1}{3} = p_3$
4		3	$\sum \mu_i \beta_{ij} \beta_j = \frac{1}{6} - \gamma + \gamma^2 = p_4$
5		4	$\sum \mu_i \alpha_i^3 = \frac{1}{4} = p_5$
6		4	$\sum \mu_i \alpha_i \alpha_{ik} \beta_k = \frac{1}{8} - \frac{\gamma}{3} = p_6$
7		4	$\sum \mu_i \beta_{ik} \alpha_k^2 = \frac{1}{12} - \frac{\gamma}{3} = p_7$
8		4	$\sum \mu_i \beta_{ik} \beta_{kl} \beta_l = \frac{1}{24} - \frac{\gamma}{2} + \frac{3\gamma^2}{2} - \gamma^3 = p_8$
9		5	$\sum \mu_i \alpha_i^4 = \frac{1}{5} = p_9$

Table 2 (continued)

Number	Tree	$\rho(t)$	Condition
10		5	$\sum \mu_i \alpha_i^2 \alpha_{ik}\beta_k = \frac{1}{10}-\frac{\gamma}{4}=p_{10}$
11		5	$\sum \mu_i\alpha_{ik}\beta_k\alpha_{il}\beta_l = \frac{1}{20}-\frac{\gamma}{4}+\frac{\gamma^2}{3}=p_{11}$
12		5	$\sum\mu_i\alpha_i\alpha_{ik}\alpha_k^2=\frac{1}{15}=p_{12}$
13		5	$\sum\mu_i\alpha_i\alpha_{ik}\beta_{kl}\beta_l=\frac{1}{30}-\frac{\gamma}{4}+\frac{\gamma^2}{3}=p_{13}$
14		5	$\sum\mu_i\beta_{ik}\alpha_k^3=\frac{1}{20}-\frac{\gamma}{4}=p_{14}$
15		5	$\sum\mu_i\beta_{ik}\alpha_k\alpha_{kl}\beta_l=\frac{1}{40}-\frac{5\gamma}{24}+\frac{\gamma^2}{3}=p_{15}$
16		5	$\sum\mu_i\beta_{ik}\beta_{kl}\alpha_l^2=\frac{1}{60}-\frac{\gamma}{6}+\frac{\gamma^2}{3}=p_{16}$
17		5	$\sum\mu_i\beta_{ik}\beta_{kl}\beta_{lm}\beta_m=\frac{1}{120}-\frac{\gamma}{6}+\gamma^2-2\gamma^3+\gamma^4=p_{17}$
18		6	$\sum\mu_i\alpha_i^5=\frac{1}{6}=p_{18}$
21		6	$\sum\mu_i\alpha_i^2\alpha_{ik}\alpha_k^2=\frac{1}{18}=p_{21}$
22		6	$\sum\mu_i\alpha_i^2\alpha_{ik}\beta_{kl}\beta_l=\frac{1}{36}-\frac{\gamma}{5}+\frac{\gamma^2}{4}=p_{22}$
25		6	$\sum\mu_i\alpha_i\alpha_{ik}\alpha_k^3=\frac{1}{24}=p_{25}$
27		6	$\sum\mu_i\alpha_i\alpha_{ik}\beta_{kl}\alpha_l^2=\frac{1}{72}-\frac{\gamma}{15}=p_{27}$
28		6	$\sum\mu_i\alpha_i\alpha_{ik}\beta_{kl}\beta_{lm}\beta_m=\frac{1}{144}-\frac{\gamma}{10}+\frac{3\gamma^2}{8}-\frac{\gamma^3}{3}=p_{28}$
29		6	$\sum\mu_i\beta_{ik}\alpha_k^4=\frac{1}{30}-\frac{\gamma}{5}=p_{29}$
34		6	$\sum\mu_i\beta_{ik}\beta_{kl}\alpha_l^3=\frac{1}{120}-\frac{\gamma}{10}+\frac{\gamma^2}{4}=p_{34}$
36		6	$\sum\mu_i\beta_{ik}\beta_{kl}\beta_{lm}\alpha_m^2=\frac{1}{360}-\frac{\gamma}{20}+\frac{\gamma^2}{4}-\frac{\gamma^3}{3}=p_{36}$
37		6	$\sum\mu_i\beta_{ik}\beta_{kl}\beta_{lm}\beta_{mn}\beta_n=\frac{1}{720}-\frac{\gamma}{24}+\frac{5\gamma^2}{12}-\frac{5\gamma^3}{3}+\frac{5\gamma^4}{2}-\gamma^5=p_{37}$

4. Study of Stability

When we apply method (5) to the test equation

$$y'=\lambda y, \qquad y(0)=1, \qquad h\lambda=z$$

we obtain

$$g_i=\frac{z}{1-\gamma z}\Big(1+\sum_j \beta_{ij}g_j\Big), \qquad \vec{g}=\frac{z}{1-\gamma z}(\vec{1}+B\vec{g})$$

using matrix notation with obvious definitions. Because of $B^s = 0$ we have

$$\vec{g} = \sum_{k=1}^{s} \left(\frac{z}{1-\gamma z}\right)^k B^{k-1} \vec{1}.$$

So we obtain finally from (5a)

$$\vec{u} = \vec{1} + \sum_{k=1}^{s} \left(\frac{z}{1-\gamma z}\right)^k A B^{k-1} \vec{1} \tag{15}$$

and

$$y_1 = R(z) = 1 + \sum_{k=1}^{s} \left(\frac{z}{1-\gamma z}\right)^k \vec{\mu}^T B^{k-1} \vec{1}. \tag{16}$$

Thus the stability function of method (5) is a rational function with one s-fold pole $z = 1/\gamma$

$$R(z) = \sum_{j=0}^{s} a_j z^j / (1-\gamma z)^s.$$

If $R(z)$ approximates e^z of order at least s, then

$$(1-\gamma z)^s e^z - \sum_{j=0}^{s} a_j z^j = O(z^{s+1}) \qquad \text{for } z \to 0.$$

An expansion of the left hand term leads to the following Proposition:

9. Proposition. *If the method is at least of order s, then*

$$R(z) = \left(\sum_{j=0}^{s} z^j \sum_{i=0}^{j} \binom{s}{i} \frac{(-\gamma)^i}{(j-i)!}\right) (1-\gamma z)^s.$$

Remark. In the above formula, the coefficients are generalized Laguerre polynomials in $1/\gamma$. This result can also be obtained from the expansion (see [17])

$$e^z = 1 + \sum_{j=0}^{\infty} \frac{(-\gamma)^j L_j^{(1)}(1/\gamma)}{j+1} (z/(1-\gamma z))^{j+1}.$$

The linear stability of the method thus depends on γ only. The following stability domains are given in [16]:

Table 3

	$s=5$	$s=6$
A-stable	$0.246506 \leqq \gamma \leqq 0.361801$ $0.420785 \leqq \gamma \leqq 0.47328$	$0.284065 \leqq \gamma \leqq 0.54090$
$A(\alpha)$-stable $(0<\alpha<\pi/2)$	$0.138197 \leqq \gamma \leqq 0.144646$ $0.47328 \leqq \gamma$	$0.101143 \leqq \gamma \leqq 0.101464$ $0.166667 \leqq \gamma \leqq 0.181912$ $0.54090 \leqq \gamma$

Since, roughly, smaller values of γ give better error constants but increase instability, there is no optimal choice which optimizes simultaneously error constant and stability. In order to achieve also good stability at infinity ($R(\infty)=0$), we have finally selected the following values:

Table 4

s	γ	Name of method	A-stable	$A(\alpha)$-stable	$R(\infty)=0$	Small error constant
5	0.278053841136	ROW5A	Yes	Yes	Yes	No
5	0.141127125787	ROW5B	No	Yes	Yes	Yes
6	0.334142367068	ROW6A	Yes	Yes	Yes	No
6	0.173155868427	ROW6B	No	Yes	Yes	Yes
6	0.101212	ROW6C	No	Yes	No	Very small

5. Construction of Methods of Order 5

Although there are methods of order 4 with $s=3$ (see [13]), we have the following negative results for $s=4$:

10. Theorem. *There exists no method of order* 5 *with* $s=4$.

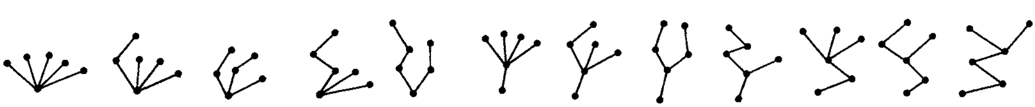
If we take $s=5$ then it holds that

11. Theorem. *There exist methods of order* 5 *with* $s=5$ *where* γ, α_3, α_4, α_5, β_2, β_3, β_4, α_{54} *are free parameters.*

For proofs of these two Theorems see [14].

Because of the great number of free parameters in this theorem, we prefer to prove instead the following result:

12. Theorem. *There exist methods of order* 5 *with* $s=5$ *that satisfy in addition the* 6*-th order conditions for the trees*



Here, γ, α_3, *and* α_4 *are, in general, free parameters.*

Proof. a) Having chosen γ, α_3 and α_4, we put $\alpha_5=1-\gamma$, $\alpha_2=2\gamma$ in order to satisfy (12) for $i=2$ and (13) for $i=5$.

b) Equations 1, 3, 5, 9, 18 of Table 2 constitute a, in general, regular linear system for the computation of $\mu_1, \mu_2, \ldots, \mu_5$.

c) If we put $x_k=\sum_{i=k+1}^{s} \mu_i \beta_{ik}$ $(k=2, 3, 4)$, Eqs. 7, 14, 29 become

$$\begin{pmatrix} \alpha_2^3 & \alpha_3^3 & \alpha_4^3 \\ \alpha_2^4 & \alpha_3^4 & \alpha_4^4 \\ \alpha_2^5 & \alpha_3^5 & \alpha_4^5 \end{pmatrix} \begin{pmatrix} x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} p_7 \\ p_{14} \\ p_{29} \end{pmatrix}$$

and allow to compute x_2, x_3, x_4 and at the moment $\beta_{54}=x_4/\mu_5$. Equations 16 and 34 now become

$$\begin{pmatrix} x_3\alpha_2^2 & x_4\alpha_2^2 & x_4\alpha_3^2 \\ x_3\alpha_2^3 & x_4\alpha_2^3 & x_4\alpha_3^3 \end{pmatrix}\begin{pmatrix}\beta_{32}\\ \beta_{42}\\ \beta_{43}\end{pmatrix}=\begin{pmatrix}p_{16}\\ p_{34}\end{pmatrix}.$$

Multiplying the first line by α_2 and subtracting, we get

$$\beta_{43}=(p_{34}-\alpha_2 p_{16})/(x_4\alpha_3^2(\alpha_3-\alpha_2)) \quad \text{and} \quad \beta_{53}=(x_3-\mu_4\beta_{43})/\mu_5.$$

d) Equations 36, 16 and the definition of x_2 give

$$\begin{pmatrix} \mu_5\beta_{54}\beta_{43}\alpha_2^2 & 0 & 0 \\ x_3\alpha_2^2 & x_4\alpha_2^2 & 0 \\ \mu_3 & \mu_4 & \mu_5 \end{pmatrix}\begin{pmatrix}\beta_{32}\\ \beta_{42}\\ \beta_{52}\end{pmatrix}=\begin{pmatrix} p_{36} \\ p_{16}-x_4\beta_{43}\alpha_3^2 \\ x_2 \end{pmatrix}$$

to compute β_{32}, β_{42}, β_{52}.

e) Equations 17, 8, 4, 2 give

$$\begin{pmatrix} x_4\beta_{43}\beta_{32} & 0 & 0 & 0 \\ x_3\beta_{32}+x_4\beta_{42} & x_4\beta_{43} & 0 & 0 \\ x_2 & x_3 & x_4 & 0 \\ \mu_2 & \mu_3 & \mu_4 & \mu_5 \end{pmatrix}\begin{pmatrix}\beta_2\\ \beta_3\\ \beta_4\\ \beta_5\end{pmatrix}=\begin{pmatrix}p_{17}\\ p_8\\ p_4\\ p_2\end{pmatrix}$$

to compute β_2, β_3, β_4, β_5, and thus β_{31}, β_{41}, β_{51} by (10).

f) If we put $w_i=\sum_{k=2}^{i-1}\beta_{ik}\beta_k$ $(i=3, \ldots, s)$, Eqs. 13 and 22 give

$$\begin{pmatrix} \mu_4\alpha_4 w_3 & \mu_5\alpha_5 w_3 & \mu_5\alpha_5 w_4 \\ \mu_4\alpha_4^2 w_3 & \mu_5\alpha_5^2 w_3 & \mu_5\alpha_5 w_4 \end{pmatrix}\begin{pmatrix}\alpha_{43}\\ \alpha_{53}\\ \alpha_{54}\end{pmatrix}=\begin{pmatrix}p_{13}\\ p_{22}\end{pmatrix}.$$

Multiplying the last line with α_5 and subtracting we obtain

$$\alpha_{43}=(p_{22}-\alpha_5 p_{13})/(\mu_4\alpha_4 w_3(\alpha_4-\alpha_5)).$$

g) Equations (12) for $i=3, 4$ give $\alpha_{32}=\alpha_3(\alpha_3/2-\gamma)/\beta_2$,

$$\alpha_{42}=(\alpha_4(\alpha_4/2-\gamma)-\alpha_{43}\beta_3)/\beta_2.$$

h) Finally Eq. 12, 13 and (12) for $i=5$ become

$$\begin{pmatrix} \mu_5\alpha_5\alpha_2^2 & \mu_5\alpha_5\alpha_3^2 & \mu_5\alpha_5\alpha_4^2 \\ 0 & w_3 & w_4 \\ \beta_2 & \beta_3 & \beta_4 \end{pmatrix}\begin{pmatrix}\alpha_{52}\\ \alpha_{53}\\ \alpha_{54}\end{pmatrix}=\begin{pmatrix}d_1\\ d_2\\ d_3\end{pmatrix}$$

where $d_1=1/15-\mu_3\alpha_3\alpha_{32}\alpha_2^2-\mu_4\alpha_4(\alpha_{42}\alpha_2^2+\alpha_{43}\alpha_3^2)$,

$$d_2=(p_{13}-\mu_4\alpha_4\alpha_{43}\beta_{32}\beta_2)/(\mu_5\alpha_5), \qquad d_3=\alpha_5(\alpha_5/2-\gamma),$$

to compute α_{52}, α_{53}, α_{54} and thus α_{21}, α_{31}, α_{41}, α_{51} by using (10). The validity of all other stated order conditions is now assured by Theorem 5. $\square$

Numerical computations have led us to the following two choices of the free parameters α_3, α_4:

Table 5

Method	γ	α_3	α_4	Quality
ROW5A	0.278053841136	0.725	0.794	A-stable and L-stable
ROW5B	0.141127125787	0.8	0.6	$A(72°)$-stable, much smaller error constant

The coefficients which result from this choice and the procedure described in the foregoing proof followed by the back-transformations (5d) are presented for ROW5 B in Table 8 below. Numerical results are given in Sect. 7.

6. Construction of Methods of Order 6

Because of Theorem 10 we have no hope to obtain formulas of order 6 with $s=5$. We thus prove:

13. Theorem. *There exist methods of order* 6 *with* $s=6$. *Here* γ, α_3, α_4, α_5, α_{63} *are in general free parameters.*

Proof. Having chosen the free parameters, we obtain from (12), $i=2$ $\alpha_2=2\gamma$ and from (13) with $k=6$ $\alpha_6=1-\gamma$. If we further sum Eqs. (13) over k, we obtain from Eq. 1, 2 of Table 1

$$\sum \mu_k \alpha_k = \sum \mu_k - \sum_{i,k} \mu_i \beta'_{ik} = 1 - 1/2 = 1/2. \tag{18}$$

b) The coefficients μ_i $(i=1, \dots, 6)$ are now obtained from the linear equations 1, (18), 3, 5, 9, 18. Further, Eq. (13) for $k=5$ gives $\beta_{65}=\mu_5(1-\alpha_5)/\mu_6$. If we choose

$$\alpha_4 = \int_0^1 t^2(t-\alpha_2)(t-\alpha_3)(t-\alpha_5)(t-\alpha_6)\,dt \Bigg/ \int_0^1 t(t-\alpha_2)(t-\alpha_3)(t-\alpha_5)(t-\alpha_6)\,dt \tag{19}$$

then by orthogonality one more order condition of order 7 is satisfied.

c) We use the abbreviations

$$\left.\begin{aligned} &x_k = \sum_i \mu_i \beta_{ik}, \quad y_k = \sum_i x_i \beta_{ik}, \quad z_k = \sum_i y_i \beta_{ik}, \\ &w_i = \sum_k \beta_{ik} \beta_k, \quad u_k = \sum_i \mu_i \alpha_i \alpha_{ik} \end{aligned}\right\} \qquad (i, k = 1, \dots, 6).$$

Then Eqs. 16, 17 and the 7-th order condition

$$\sum \mu_i \beta_{ik} \beta_{kl} \alpha_l^4 = \frac{1}{210} - \frac{\gamma}{15} + \frac{\gamma^2}{5} = p_{77}$$

become

$$\begin{pmatrix} \alpha_2^2 & \alpha_3^2 & \alpha_4^2 \\ \alpha_2^3 & \alpha_3^3 & \alpha_4^3 \\ \alpha_2^4 & \alpha_3^4 & \alpha_4^4 \end{pmatrix} \begin{pmatrix} y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} p_{16} \\ p_{34} \\ p_{77} \end{pmatrix}$$

to obtain y_2, y_3, y_4.

d) We suppose now that w_3 is known (see below, point h)) and compute z_3, z_2 from Eqs. 37, 36

$$\begin{pmatrix} w_3 & 0 \\ \alpha_3^2 & \alpha_2^2 \end{pmatrix} \begin{pmatrix} z_3 \\ z_2 \end{pmatrix} = \begin{pmatrix} p_{37} \\ p_{36} \end{pmatrix},$$

compute w_4, w_5 from 17, 8

$$\begin{pmatrix} y_4 & 0 \\ x_4 & x_5 \end{pmatrix} \begin{pmatrix} w_4 \\ w_5 \end{pmatrix} = \begin{pmatrix} p_{17} - y_3 w_3 \\ p_8 - x_3 w_3 \end{pmatrix},$$

compute β_{54}, β_{64} from y_4 and x_4

$$\begin{pmatrix} x_5 & 0 \\ \mu_5 & \mu_6 \end{pmatrix} \begin{pmatrix} \beta_{54} \\ \beta_{64} \end{pmatrix} = \begin{pmatrix} y_4 \\ x_4 \end{pmatrix},$$

and compute β_{43}, β_{53}, β_{63} from z_3, y_3, x_3

$$\begin{pmatrix} y_4 & 0 & 0 \\ x_4 & x_5 & 0 \\ \mu_4 & \mu_5 & \mu_6 \end{pmatrix} \begin{pmatrix} \beta_{43} \\ \beta_{53} \\ \beta_{63} \end{pmatrix} = \begin{pmatrix} z_3 \\ y_3 \\ x_3 \end{pmatrix}.$$

e) Equations 12, 13, 25, 28

$$\begin{pmatrix} \alpha_2^2 & \alpha_3^2 & \alpha_4^2 & \alpha_5^2 \\ \alpha_2^3 & \alpha_3^3 & \alpha_4^3 & \alpha_5^3 \\ 0 & w_3 & w_4 & w_5 \\ 0 & 0 & \beta_{43} w_3 & \beta_{53} w_3 + \beta_{54} w_4 \end{pmatrix} \begin{pmatrix} u_2 \\ u_3 \\ u_4 \\ u_5 \end{pmatrix} = \begin{pmatrix} p_{12} \\ p_{25} \\ p_{13} \\ p_{28} \end{pmatrix}$$

give u_2, u_3, u_4, u_5.

f) Equation 27 and the definition of z_2, y_2, x_2 give

$$\begin{pmatrix} y_3 & y_4 & 0 & 0 \\ x_3 & x_4 & x_5 & 0 \\ u_3 \alpha_2^2 & u_4 \alpha_2^2 & u_5 \alpha_2^2 & 0 \\ \mu_3 & \mu_4 & \mu_5 & \mu_6 \end{pmatrix} \begin{pmatrix} \beta_{32} \\ \beta_{42} \\ \beta_{52} \\ \beta_{62} \end{pmatrix} = \begin{pmatrix} z_2 \\ y_2 \\ q \\ x_2 \end{pmatrix}$$

to compute $\beta_{32}, \beta_{42}, \beta_{52}, \beta_{62}$. Here $q = p_{27} - u_4 \beta_{43} \alpha_3^2 - u_5(\beta_{53} \alpha_3^2 + \beta_{54} \alpha_4^2)$.

g) The definition of w_3, w_4, w_5 and Eqs. 4 and 2 yield

$$\begin{pmatrix} \beta_{32} & 0 & 0 & 0 & 0 \\ \beta_{42} & \beta_{43} & 0 & 0 & 0 \\ \beta_{52} & \beta_{53} & \beta_{54} & 0 & 0 \\ x_2 & x_3 & x_4 & x_5 & 0 \\ \mu_2 & \mu_3 & \mu_4 & \mu_5 & \mu_6 \end{pmatrix} \begin{pmatrix} \beta_2 \\ \beta_3 \\ \beta_4 \\ \beta_5 \\ \beta_6 \end{pmatrix} = \begin{pmatrix} w_3 \\ w_4 \\ w_5 \\ p_4 \\ p_2 \end{pmatrix}$$

to obtain $\beta_2, \beta_3, \beta_4, \beta_5, \beta_6$ and by (10) $\beta_{21}, \beta_{31}, \beta_{41}, \beta_{51}, \beta_{61}$.

h) So far we have obtained all u_i and all β_i. Now Eq. 6 of Table 2

$$\sum_{i=2}^{5} u_i\beta_i - 1/8 + \gamma/3 = 0 \qquad (20)$$

is used to adjust the value for w_3, which has been left open above. So all computations from point d) to g) are repeated several times, until (usually two) solutions of Eq. (20) have been found by a root finding Regula-Falsi algorithm.

i) The Eqs. (12) for $i=3, 4, 5, 6$ and the definitions of u_2, u_3, u_4, u_5 give eight equations

$$\begin{pmatrix} \beta_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \beta_2 & \beta_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \beta_2 & \beta_3 & \beta_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \beta_2 & \beta_3 & \beta_4 & \beta_5 \\ \mu_3\alpha_3 & \mu_4\alpha_4 & 0 & \mu_5\alpha_5 & 0 & 0 & \mu_6\alpha_6 & 0 & 0 & 0 \\ 0 & 0 & \mu_4\alpha_4 & 0 & \mu_5\alpha_5 & 0 & 0 & \mu_6\alpha_6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu_5\alpha_5 & 0 & 0 & \mu_6\alpha_6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mu_6\alpha_6 \end{pmatrix}$$

$$\begin{pmatrix} \alpha_{32} \\ \alpha_{42} \\ \alpha_{43} \\ \alpha_{52} \\ \alpha_{53} \\ \alpha_{54} \\ \alpha_{62} \\ \alpha_{63} \\ \alpha_{64} \\ \alpha_{65} \end{pmatrix} = \begin{pmatrix} \alpha_3(\alpha_3/2-\gamma) \\ \alpha_4(\alpha_4/2-\gamma) \\ \alpha_5(\alpha_5/2-\gamma) \\ \alpha_6(\alpha_6/2-\gamma) \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{pmatrix}.$$

The lines of this matrix are linearly dependent: If the lines 1 to 4 are multiplied by $-\mu_i\alpha_i$ and lines 5 to 8 are multiplied by β_i and added, we obtain zero. Therefore there is a solution only if the right hand side has the same linear dependence

$$\sum_{i=2}^{5} \mu_i\beta_i - \sum_{i=3}^{6} \mu_i\alpha_i^2(\alpha_i/2-\gamma) = 0.$$

But this, due to Eqs. 3 and 5, is just (20). So we delete one (the fifth) equation, add Eqs. 21, 22 and move the terms with α_{63} to the right. This then gives a regular 7×7 system to compute α_{ik} $(k=2, 5)$, and, by (10), α_{i1}.

The free parameter α_{63} can be used to minimize the magnitudes of a_{ij}, c_{ij} and the error constant by a Fibonacci search. $\square$

Extensive numerical computations suggested the following choices of the free parameters:

Table 6

	ROW6A	ROW6B	ROW6C
γ	0.33414236706805043	0.17315586842719120	0.101212
α_3	0.82	0.74	0.64
α_5	0.90	0.58	0.38
α_{63}	−0.11139	−0.342242	0.10009
w_3	−0.1258668298991528	0.19866532271607364	0.20310963112766355
Stability angle	90°	85.74°	26.78°
Error constant	3.575/7!	0.4441/7!	0.04077/7!

A Fortran program which executes, for γ, α_3, α_5 given, the procedure of the above proof can be obtained from the authors.

7. Numerical Results

All 5 constructed methods have been built into subroutines, available from the authors. Thereby, the automatic adjustement of the step size is done with Richardson extrapolation: For a given initial value y_0 and step size h, the program computes the solutions y_1 and y_2 of two successive steps with step size h and the solution $\hat{y}_2$ with one large step from y_0 with step size $2h$. Then the local error of y_2 is extrapolated as

$$\mathrm{ERR} = \max_{i=1,n} \left(|y_{2,i} - \hat{y}_{2,i}|/(2^p - 1) \max(1, |y_{2,i}|)\right).$$

Here, for $|y_{2,i}| \leqq 1$ we use the absolute error, and for $|y_{2,i}| \geqq 1$ the relative error. This is, of course, not the best choice for all problems. When TOL is the allowed local tolerance, the new step size is computed as

$$h_{\mathrm{new}} = h \cdot \min(3.2, \max(0.5, 0.9(\mathrm{TOL}/\mathrm{ERR})^{1/p})).$$

Here again, the safety bounds 3.2 and 0.5 may not be the best. For $\mathrm{ERR} \leq \mathrm{TOL}$, h_{new} is used to continue the computation from the new initial point y_2, otherwise both steps are recomputed from y_0 with this new step size.

In order to study, which of the choices of γ was the best, we ran the three ROW6 methods on all 25 stiff test examples of Enright-Hull-Lindberg [11], and counted the total number of steps. The results are shown in Fig. 4. Method ROW6C was the best on linear problems with real eigenvalues (class A), but did not behave well on problems with complex eigenvalues (class B) due to lack of stability, neither on nonlinear problems (class D). Clearly superior was the "compromise method" ROW6B.

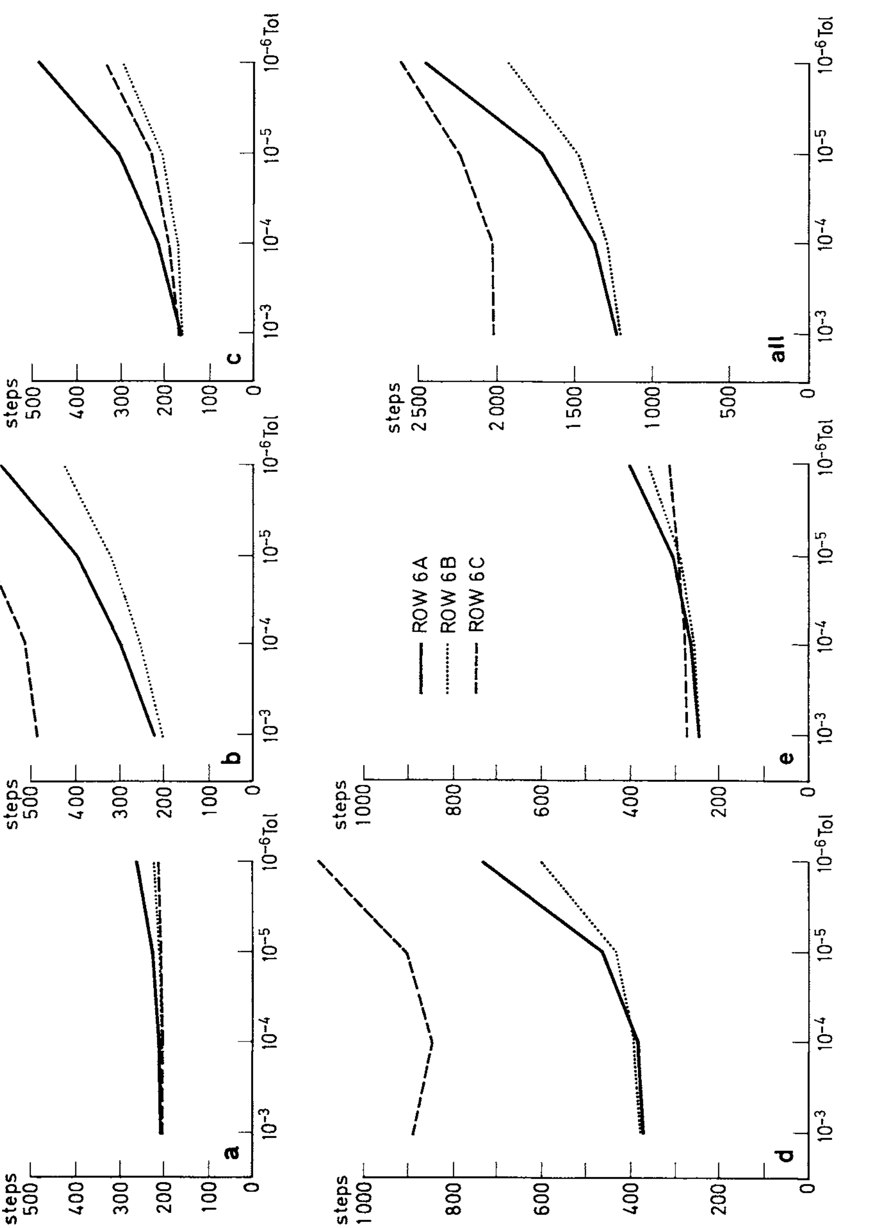


Fig. 4. Number of computed steps of methods ROW6A, B, C

Finally, in Fig. 5, the actual computing times as a function of TOL of the programs ROW5B and ROW6B are compared with the fourth order ROW method of Kaps and Rentrop [6] as implemented in [12] (ROW4A) and Hindmarsh's implementation of GEAR's BDF formulas. GEAR is usually the fastest program, but is not sufficiently stable for complex eigenvalues (class B,

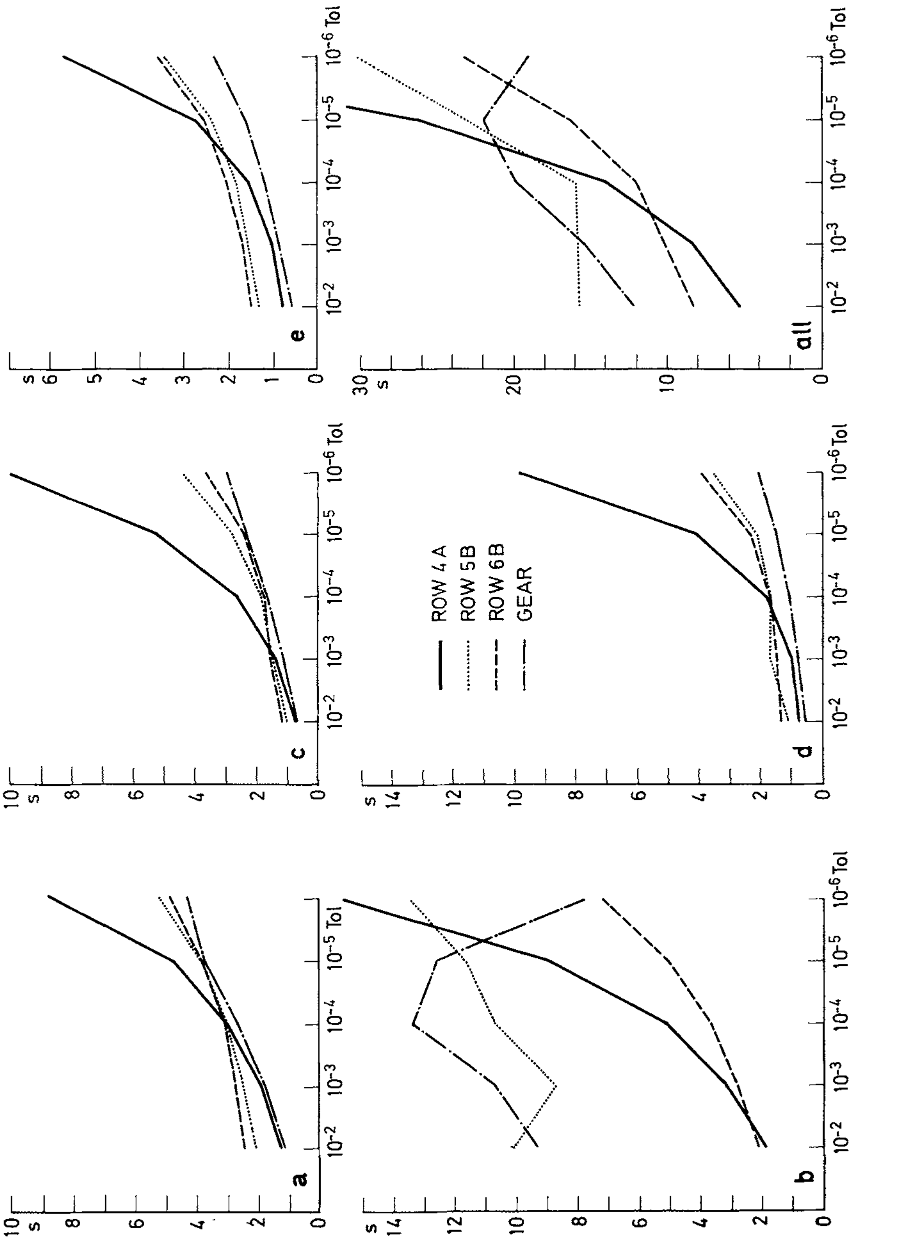


Fig. 5. Computing times on Univac 1108 for methods GEAR, ROW4A, ROW5B and ROW6B for problems of Enright et al.

especially problem B5), so that - overall - ROW4A is best for 10^{-2}, 10^{-3}, and ROW6B us best for 10^{-4} and 10^{-5}.

As to the *actual errors*, ROW4A is by far the most reliable code, as can be seen from the following table, which indicates the number of numerical results with large error (out of 97):

Table 7. Number of numerical results with large error

	Error > TOL					Error > 10.TOL				
	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}
ROW4A	1	0	2	2	2	0	0	0	0	0
ROW5B	7	5	7	7	9	4	2	2	0	2
ROW6B	2	3	6	8	8	2	1	4	3	2
GEAR	8	12	11	11	12	1	1	1	3	3

Table 8. Coefficients of ROW5B

a_{21}	=	0.28225425157410630D+00
c_{21}	=	−0.81524951688460885D+00
a_{31}	=	0.57116380169300584D+00
c_{31}	=	0.81127189717323099D+01
a_{32}	=	0.12386230035678339D+01
c_{32}	=	0.64300627424554704D+00
a_{41}	=	0.72285966684392441D+00
c_{41}	=	0.18891319022399990D−01
a_{42}	=	0.97672836707474073D+00
c_{42}	=	−0.37493862667874616D+01
a_{43}	=	−0.32856006264202144D−01
c_{43}	=	0.95094153717403742D−01
a_{51}	=	0.67849717523250110D+00
c_{51}	=	0.53507619725099805D+01
a_{52}	=	0.20208927497707465D+01
c_{52}	=	−0.25460873945213962D+01
a_{53}	=	−0.10701369811124179D+00
c_{53}	=	0.41864844423231233D+00
a_{54}	=	0.66019768386713535D+00
c_{54}	=	−0.33062805583808154D+01
m_1	=	0.77900694405566295D+00
m_2	=	0.37121621947171690D+01
m_3	=	−0.73417673328703555D+00
m_4	=	0.24040545624571883D+01
m_5	=	0.59299247626627483D+00
A_1	=	0.00000000000000000D+00
B_1	=	0.14112712578705315D+00
A_2	=	0.28225425157410630D+00
B_2	=	0.26073304669844646D−01
A_3	=	0.80000000000000000D+00
B_3	=	0.13028171350787572D+01
A_4	=	0.60000000000000000D+00
B_4	=	0.16992460579297673D+00
A_5	=	0.85887287421294685D+00
B_5	=	0.81348381758071946D+00

Table 9. Coefficients of ROW6A

a_{21}	=	0.66828473413610087D+000
c_{21}	=	−0.58308828523185086D+001
a_{31}	=	0.58524803895736580D+000
c_{31}	=	−0.40175939515896193D+001
a_{32}	=	−0.48594008221492802D−001
c_{32}	=	0.43970131925236112D+000
a_{41}	=	−0.61719233202999775D+000
c_{41}	=	0.77228006257490299D+001
a_{42}	=	−0.83995264476522158D+000
c_{42}	=	0.43368108251435758D+001
a_{43}	=	0.62641917900148600D+000
c_{43}	=	−0.28219574578033366D+001
a_{51}	=	0.35406887484552165D+001
c_{51}	=	−0.10516225114542007D+001
a_{52}	=	0.65991497772646308D+000
c_{52}	=	−0.58853585181331353D+000
a_{53}	=	−0.63661180895697222D+000
c_{53}	=	0.20433794587212771D+001
a_{54}	=	−0.11945984675295562D+001
c_{54}	=	0.50098631723809151D+001
a_{61}	=	0.80783664328582613D+000
c_{61}	=	−0.67357785372199458D+001
a_{62}	=	0.10194631616818569D+000
c_{62}	=	−0.53593889506199845D+000
a_{63}	=	−0.78396778850607012D−001
c_{63}	=	0.38622517020810987D+000
a_{64}	=	−0.44341977375427388D−001
c_{64}	=	0.21066472713931598D+000
a_{65}	=	0.13074732797453325D−001
c_{65}	=	−0.53546655670373728D−001
m_1	=	0.11358660043232931D+002
m_2	=	−0.69896898855829058D+001
m_3	=	−0.45967580421042947D+001
m_4	=	−0.37220984696531517D+001
m_5	=	0.96012685868421520D+000
m_6	=	0.12953396234292936D+002
A_1	=	0.00000000000000000
B_1	=	0.33414236706805043D+000
A_2	=	0.66828473413610087D+000
B_2	=	−0.16142026313021616D+001
A_3	=	0.82000000000000000D+000
B_3	=	−0.17180730123585805D+001
A_4	=	0.21963625075792513D+000
B_4	=	0.76249475341993402D+000
A_5	=	0.89999999999999999D+000
B_5	=	0.12420861346966895D+001
A_6	=	0.66585763293194957D+000
B_6	=	−0.16208944937998730D+001

Table 10. Coefficients of ROW6B

a_{21}	= 0.34631173685438241D+000
c_{21}	= −0.63453397891179372D+000
a_{31}	= 0.51484422823733024D+000
c_{31}	= 0.36437911365480913D+001
a_{32}	= 0.61607853745814515D+000
c_{32}	= 0.12945713592535053D+001
a_{41}	= 0.42083594880532555D+000
c_{41}	= 0.69161953050956585D−001
a_{42}	= 0.12398256101276536D+000
c_{42}	= −0.12905884218846234D+000
a_{43}	= −0.43663557947609954D−002
c_{43}	= −0.40532167899763093D−001
a_{51}	= 0.44508808952624152D+000
c_{51}	= 0.17583309748309236D+001
a_{52}	= 0.14790956438776313D+000
c_{52}	= 0.17092158755220803D+001
a_{53}	= −0.10863189236472590D−001
c_{53}	= −0.54015868028686558D−001
a_{54}	= 0.16749655714649715D+000
c_{54}	= −0.14204573489819585D+001
a_{61}	= −0.78286965861140857D+000
c_{61}	= 0.92366768689092273D+001
a_{62}	= −0.16763611643856503D+001
c_{62}	= 0.11681533450127634D+002
a_{63}	= −0.54599770789200043D+000
c_{63}	= 0.24468706426428219D+001
a_{64}	= −0.42431494939094088D+000
c_{64}	= 0.28555063127446144D+001
a_{65}	= 0.27503664994042264D+001
c_{65}	= −0.12600541876984773D+002
m_1	= −0.67246858827422954D+001
m_2	= −0.12998203944959025D+002
m_3	= −0.41709683120954452D+001
m_4	= −0.20786455336141339D+001
m_5	= 0.15638447165125274D+002
m_6	= 0.10493031673621379D+001
A_1	= 0.00000000000000000
B_1	= 0.17315586842719120D+000
A_2	= 0.34631173685438241D+000
B_2	= 0.63282586262158533D−001
A_3	= 0.74000000000000000D+000
B_3	= 0.88602351075795778D+000
A_4	= 0.44380509942047506D+000
B_4	= 0.14105203545498545D+000
A_5	= 0.58000000000000000D+000
B_5	= 0.33756706706153310D+000
A_6	= 0.82684413157280881D+000
B_6	= 0.82901025130889673D+000

Table 11. Coefficients of ROW6C

a_{21}	= 0.20242400000000000D+000
c_{21}	= −0.83711460854632873D+000
a_{31}	= 0.44621654865643444D+000
c_{31}	= 0.81095997353033715D+001
a_{32}	= 0.11896920258725748D+001
c_{32}	= 0.52957481214971646D+001
a_{41}	= 0.18391895721753722D+000
c_{41}	= 0.23526327774704726D+002
a_{42}	= 0.11534153564796522D+001
c_{42}	= 0.22110500878185557D+002
a_{43}	= 0.40800443372639369D−001
c_{43}	= 0.94390106357306037D−001
a_{51}	= 0.39787492846073422D+000
c_{51}	= −0.11466903149967049D+002
a_{52}	= 0.87515065537444452D+000
c_{52}	= −0.16940427049116608D+002
a_{53}	= 0.10127597282496418D+001
c_{53}	= −0.79770360614040555D+001
a_{54}	= −0.35294772495604536D+000
c_{54}	= 0.26848794528360615D+001
a_{61}	= −0.22008184569010367D+000
c_{61}	= 0.83213754445976225D+001
a_{62}	= 0.25236688996602158D+001
c_{62}	= −0.17359074625123762D+001
a_{63}	= 0.39879272204714589D+001
c_{63}	= −0.23526586513232128D+002
a_{64}	= −0.10954283528816804D+001
c_{64}	= 0.62751642468284353D+001
a_{65}	= 0.49005800407447388D+000
c_{65}	= −0.33258470695305451D+001
m_1	= −0.68686360211706425D+000
m_2	= 0.36389829748032085D+001
m_3	= 0.78330677400851241D+001
m_4	= −0.21841333005666802D+001
m_5	= 0.10310923075194031D+001
m_6	= 0.28470488298984924D+000
A_1	= 0.00000000000000000
B_1	= 0.10121200000000000D+000
A_2	= 0.20242400000000000D+000
B_2	= 0.16485956239808977D−001
A_3	= 0.64000000000000000D+000
B_3	= 0.10093062801975777D+001
A_4	= 0.77866363990435074D+000
B_4	= 0.29421399637863861D+001
A_5	= 0.37999999999999998D+000
B_5	= −0.14906367986296386D+001
A_6	= 0.89878799999999989D+000
B_6	= 0.58932697599267412D+000

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