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Generalized Runge-Kutta Methods of Order Four with Stepsize Control for Stiff Ordinary Differential Equations

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Summary. Generalized $A(\alpha)$-stable Runge-Kutta methods of order four with stepsize control are studied. The equations of condition for this class of semi-implicit methods are solved taking the truncation error into consideration. For application an A-stable and an $A(89.3°)$-stable method with small truncation error are proposed and test results for 25 stiff initial value problems for different tolerances are discussed.

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1. Introduction

Initial value problems with strongly decreasing and increasing solution components are called stiff problems. They mainly appear in chemical kinetics, electric circuits and control theory. Usual integration routines as compared in Diekhoff et al. [6], Enright et al. [7] fail, because of the different growth of the solution components. New stability requirements like A-stability have been introduced to overcome these problems, see Dahlquist [5], Grigorieff [10].

The present report is concerned with generalized Runge-Kutta methods of order four with three function evaluations per step. A stepsize control is implemented by embedding a third order method. One evaluation of the Jacobi matrix and the solution of a linear equation system of order n is necessary per step. An A-stable and an $A(89.3°)$-stable algorithm are tested by solving 25 stiff initial value problems from Bedet, Enright, Hull [2] and Enright, Hull, Lindberg [8].

2. Generalized Runge-Kutta Methods

ROW-Methods. The autonomous initial value problem:

$$y'(x) = f(y(x)), \qquad y(x_0) = y_0 \tag{2.1}$$

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is considered in a n-dimensional real or complex space. A numerical solution of the following type is studied:

$$y_h(x_0+h)=y_0+\sum_{i=1}^{s} c_i k_i \tag{2.2}$$

$$(I-\gamma h f'(y_0))\,k_i = h f\left(y_0+\sum_{j=1}^{i-1}\alpha_{ij}k_j\right)+h f'(y_0)\sum_{j=1}^{i-1}\gamma_{ij}k_j \qquad i=1,\dots,s.$$

The coefficients γ, c_i, α_{ij}, γ_{ij} are real numbers, h denotes the stepsize, $f'(y_0)$ the Jacobi-, I the $n\times n$ identity matrix and s the number of stages. The vectors k_i ($i=1,\dots,s$) are computed by solving a system of linear equations of order n for s different right hand sides.

Method (2.2) is called Rosenbrock-Wanner method, short ROW-method. The first who seemed to have studied similar formulas was Rosenbrock [18]. Wanner [20] introduced the coefficients γ_{ij} and proposed the theory of Butcher series [11] for derivation of the equations of condition. In [13] and Wolfbrandt [21] these methods are called modified Rosenbrock methods, in Nørsett, Wolfbrandt [17] ROW-methods.

For $\gamma=\gamma_{ij}=0$ the ROW-methods reduce to usual Runge-Kutta methods. Therefore ROW-methods can be considered as generalized Runge-Kutta methods.

Stability Properties of ROW-Methods. To study the stability properties of ROW-methods, the scalar test differential equation is used:

$$y'=\lambda y, \quad y(x_0)=y_0; \quad \lambda\in\mathbb{C},\ y_0\in\mathbb{C},\ y\colon \mathbb{R}\to\mathbb{C}$$

Since $f'(y)=\lambda$, it holds: $k_i=R_i(z)\,y_0$, $z=\lambda h$, where $R_i(z)$ are rational functions with denominator $(1-\gamma z)^i$ and degree of numerator $\leqq i$. Thus the numerical solution y_h is:

$$y_h=R(z)\,y_0 \tag{2.3}$$

with the stability function: $R(z)=1+\sum_{i=1}^{s} c_i R_i(z)=\dfrac{P(z)}{Q(z)}$. For a rational approximation (2.3) of order p holds:

Proposition (2.4). The stability function of a ROW-method with order $p\geqq s$ is given by

$$R(z)=\frac{1}{(1-\gamma z)^s}\sum_{k=0}^{s} L_k^{(s-k)}\left(\frac{1}{\gamma}\right)(-\gamma z)^k,$$

where

$$L_k^{(\alpha)}(x)=\sum_{i=0}^{n}(-1)^i\binom{n+\alpha}{n-i}\frac{x^i}{i!}$$

stands for the generalized Laguerre polynomials, see Abramowitz, Stegun [1]. $R(z)$ is a rational approximation to e^z of order $\geqq s$.

Proof. Applying Theorem 4 or Proposition 6 of Nørsett, Wanner [16] one can show that $P(z)$ is determined uniquely by $Q(z)$. In our case the symmetric polynomials S_i are:

$S_i = \binom{s}{i} \gamma^i$. It follows:

$$P(z) = \sum_{k=0}^{s} (-\gamma z)^k \sum_{i=0}^{k} (-1)^i \binom{s}{k-i} \frac{\gamma^{-i}}{i!}. \quad \blacklozenge$$

By means of the stability function one can characterize some stability properties very conveniently.

One has stability at infinity, iff:

$$\lim_{z \to \infty} |R(z)| = \left| L_s\left(\frac{1}{\gamma}\right) \right| \leqq 1, \qquad \text{where } L_s := L_s^{(0)}. \tag{2.5}$$

For $\gamma > 0$ a method (2.2) is A-stable, iff:

$$|R(iy)| \leqq 1 \qquad \text{for } y \in \mathbb{R} \tag{2.6}$$

or equivalently, iff the E-polynomial (see Nørsett [15]) satisfies:

$$E(y) = |Q(iy)|^2 - |P(iy)|^2 \geqq 0 \qquad \forall\, y \in \mathbb{R}. \tag{2.7}$$

Embedded ROW-Methods. Error estimation and stepsize control is performed using two embedded methods. A ROW-method of order 4:

$$y_h(x_0 + h) = y_0 + \sum_{i=1}^{s} c_i k_i \tag{2.8}$$

and a ROW-method of order 3:

$$\hat{y}_h(x_0 + h) = y_0 + \sum_{i=1}^{\hat{s}} \hat{c}_i k_i \qquad (\hat{s} \leqq s)$$

are combined, where the coefficients γ, γ_{ij}, α_{ij} $(i = 1, \ldots, s,\ j = 1, \ldots, i-1)$ and therefore the k_i are the same for both formulas. The result of the fourth order method is taken as initial guess for the next step. The different orders of the two formulas lead to an estimation of the local truncation error EST of the third order method, in analogy to [6] and [7]. Using this information the following stepsize control for a given tolerance TOL is proposed.

$$h_{\text{new}} := 0.9\, h_{\text{old}} \left(\frac{\text{TOL}}{\text{EST}}\right)^{\frac{1}{4}} \tag{2.9}$$

"if" h_{new} "greater" $1.5\, h_{\text{old}}$ "then" $h_{\text{new}} := 1.5\, h_{\text{old}}$

"if" h_{new} "less" $0.5\, h_{\text{old}}$ "then" $h_{\text{new}} := 0.5\, h_{\text{old}}$.

The safety factor 0.9 serves to keep h_{new} small enough to be accepted, if the truncation error in the next step is growing. The bounds 0.5 and 1.5 for the ratio of two steps are introduced to prevent a stepsize prediction, which is highly zig-zag in character. The values of the three constants are fixed by experience. EST is defined by

$$\text{EST} := \max_{i=1}^{n} \frac{|y_{i,h}(x_{\text{old}}) - \hat{y}_{i,h}(x_{\text{old}})|}{S_i},$$

where $S = (S_1, \ldots, S_n)^T$ stands for a suitable scaling vector.

$$S_i := \max(C, |y_{i,h}(x_j)|) \qquad i = 1, \ldots, n \tag{2.10}$$

$$C > 0 \quad \text{(in the following } C = 1)$$

$$x_0 \leqq x_j \leqq x_{\text{old}}, \quad x_j \text{ represents the discrete abscissa.}$$

h_{new} is accepted, if $\text{EST} \leqq \text{TOL}$, otherwise formula (2.9) is applied once more with the value EST belonging to the failed stepsize prediction. This yields a smaller h_{new}, which may be successful. Repeated application of (2.9) is terminated, if $h_{\text{new}} \leqq h_{\min}$. The minimal allowed stepsize $h_{\min}$ depends on the relative machine precision and on the interval length.

Usually one is interested in the relative precision of the achieved solution. In stiff differential equations, however, strongly decaying solution components occur, which are less interesting for the user. Therefore the mixed tolerance (2.10) is used. For the test set [8] it was sufficient to apply relative tolerance for solution components with $|y_{i,h}| \geqq 1$ and absolute tolerance for $|y_{i,h}| < 1$. Obviously the switching point for the mixed tolerance depends on the scaling factors of a problem.

For the design of (3)4-methods it is important that the fourth order method possesses good stability properties and small truncation errors. In part 3 it is shown that these requirements cannot be satisfied simultaneously. Stability conditions for the third order can be chosen weakly. The third order method is not used for step continuation, therefore truncation error investigations are important. If $R(z)$ and $\hat{R}(z)$ denote the stability function (2.3) of order 3 and 4, respectively, then for the scalar test problem:

$$y' = \lambda y, \qquad y(x_0) = y_0, \qquad \lambda \in \mathbb{C}$$

one obtains: $\text{EST} = |\hat{R}(z) - R(z)|\,|y_0|/S_1$.

This is an acceptable error estimation for $z \in \mathbb{C}^- = \{z \in \mathbb{C} / \text{Re}(z) < 0\}$, if $\sup_{z \in \mathbb{C}^-} |\hat{R}(z)|$ is not too large. Finally it should be remarked, that the stepsize control formula (2.9) has been chosen, although it represents an error-per-unit-step for the fourth order method, because the local truncation error of the fourth order method is smaller than those of the third order method.

3. Equations of Condition

The simplified equations of condition are derived in [13, 14] applying the theory of Butcher series [11]. Equations up to order 5 for y_h are listed below

$$\text{order 1:} \quad \sum c_i = 1, \tag{3.1}$$

$$\text{order 2:} \quad \sum c_i \beta_i = \tfrac{1}{2} - \gamma = P_2(\gamma), \tag{3.2}$$

$$\text{order 3:} \quad \sum c_i \alpha_i^2 = \tfrac{1}{3}, \tag{3.3}$$

$$\sum c_i \beta_{ij} \beta_j = \tfrac{1}{6} - \gamma + \gamma^2 = P_4(\gamma), \tag{3.4}$$

$$\text{order 4:} \quad \sum c_i \alpha_i^3 = \tfrac{1}{4}, \tag{3.5}$$

$$\sum c_i \alpha_i \alpha_{ik} \beta_k = \tfrac{1}{8} - \tfrac{1}{3}\gamma = P_6(\gamma), \tag{3.6}$$

$$\sum c_i \beta_{ik} \alpha_k^2 = \tfrac{1}{12} - \tfrac{1}{3}\gamma = P_7(\gamma), \tag{3.7}$$

$$\sum c_i \beta_{ik} \beta_{kl} \beta_l = \tfrac{1}{24} - \tfrac{1}{2}\gamma + \tfrac{3}{2}\gamma^2 - \gamma^3 = P_8(\gamma), \tag{3.8}$$

order 5: (for truncation error investigations)

$$\sum c_i \alpha_i^4 = \tfrac{1}{5}, \tag{3.9}$$

$$\sum c_i \alpha_i^2 \alpha_{ik} \beta_k = \tfrac{1}{10} - \tfrac{1}{4}\gamma = P_{10}(\gamma), \tag{3.10}$$

$$\sum c_i \alpha_{ik} \beta_k \alpha_{il} \beta_l = \tfrac{1}{20} - \tfrac{1}{4}\gamma + \tfrac{1}{3}\gamma^2 = P_{11}(\gamma), \tag{3.11}$$

$$\sum c_i \alpha_i \alpha_{ik} \alpha_k^2 = \tfrac{1}{15}, \tag{3.12}$$

$$\sum c_i \alpha_i \alpha_{ik} \beta_{kl} \beta_l = \tfrac{1}{30} - \tfrac{1}{4}\gamma + \tfrac{1}{3}\gamma^2 = P_{13}(\gamma), \tag{3.13}$$

$$\sum c_i \beta_{ik} \alpha_k^3 = \tfrac{1}{20} - \tfrac{1}{4}\gamma = P_{14}(\gamma), \tag{3.14}$$

$$\sum c_i \beta_{ik} \alpha_k \alpha_{kl} \beta_l = \tfrac{1}{40} - \tfrac{5}{24}\gamma + \tfrac{1}{3}\gamma^2 = P_{15}(\gamma), \tag{3.15}$$

$$\sum c_i \beta_{ik} \beta_{kl} \alpha_l^2 = \tfrac{1}{60} - \tfrac{1}{6}\gamma + \tfrac{1}{3}\gamma^2 = P_{16}(\gamma), \tag{3.16}$$

$$\sum c_i \beta_{ik} \beta_{kl} \beta_{lm} \beta_m = \tfrac{1}{120} - \tfrac{1}{6}\gamma + \gamma^2 - 2\gamma^3 + \gamma^4 = P_{17}(\gamma) \tag{3.17}$$

summation indices $i, j, k, l, m = 1, \ldots, s$,

abbreviations

$$\alpha_i = \sum \alpha_{ij}, \qquad \beta_i = \sum \beta_{ij},$$

$$\beta_{ij} = \alpha_{ij} + \gamma_{ij}, \qquad \alpha_{ij} = \gamma_{ij} = 0 \qquad \text{for } i \leqq j.$$

Remark. The order conditions for $\hat{y}_h$ are obtained by replacing c_i by $\hat{c}_i$ and s by $\hat{s}$ in the above equations. They are denoted by $(\hat{\ })$. From (3.4) and (3.8) it follows immediately, that there are no methods of order 4 with $s=2$. A-stable methods of order 4 exist for $s=3$, see [13, 14]. There is no embedded method (2.8) with $s=3$, $\hat{s} \leqq 3$, see Lemma (3.18). Nevertheless, one can construct methods with $s=4$, $\hat{s}=3$ and only three function evaluations per step, see Propositions (3.19), (3.20). In [13, 14] it is shown that there exists no five order method (2.2) with $s=4$.

Lemma (3.18). There exists no embedded method (2.8) with $s=3$, $\hat{s} \leqq 3$.

Proof. $\hat{s}=2$ is impossible, because the zeros of $P_4(\gamma)$ and $P_8(\gamma)$ are different. Let $\hat{s}=3$, then (3.1), (3.3) and (3.4) for y_h and $\hat{y}_h$ define the same linear system for the c_i, resp. $\hat{c}_i$ $(i=1,2,3)$. Due to (3.7) and (3.8) the system has a unique solution $c_i = \hat{c}_i$. ◆

Proposition (3.19). There exist embedded methods (2.8) with $s=4$, $\hat{s}=3$ and three function evaluations per step. The parameters γ, α_2, α_3, c_4 and β_{43} are free (except for special values leading to nonsolvable linear systems).

Proof. Choosing $\alpha_4 = \alpha_3$, with $\alpha_{41} = \alpha_{31}$, $\alpha_{42} = \alpha_{32}$, $\alpha_{43} = 0$, one gets a four stage method with only three function evaluations. Equations (3.1), (3.3), (3.5) determine c_1, c_2, c_3+c_4:

$$\begin{pmatrix} 1 & 1 & 1 \\ 0 & \alpha_2^2 & \alpha_3^2 \\ 0 & \alpha_2^3 & \alpha_3^3 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3+c_4 \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{3} \\ \frac{1}{4} \end{pmatrix}.$$

From (3.8) follows: $\beta_{32}\beta_2 = P_8(\gamma)/c_4\beta_{43} =: u$. Equations $(\hat{3.1})$, $(\hat{3.3})$, $(\hat{3.4})$ define $\hat{c}_1$, $\hat{c}_2$, $\hat{c}_3$:

$$\begin{pmatrix} 1 & 1 & 1 \\ 0 & \alpha_2^2 & \alpha_3^2 \\ 0 & 0 & u \end{pmatrix} \begin{pmatrix} \hat{c}_1 \\ \hat{c}_2 \\ \hat{c}_3 \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{3} \\ P_4(\gamma) \end{pmatrix}$$

(3.7) leads to: $c_3\beta_{32} + c_4\beta_{42} = (P_7(\gamma) - c_4\beta_{43}\alpha_3^2)/\alpha_2^2 = : v$. From (3.4) and $(\hat{3.2})$ one obtains β_2 and β_3:

$$\begin{pmatrix} v & c_4\beta_{43} \\ \hat{c}_2 & \hat{c}_3 \end{pmatrix} \begin{pmatrix} \beta_2 \\ \beta_3 \end{pmatrix} = \begin{pmatrix} P_4(\gamma) \\ P_2(\gamma) \end{pmatrix}$$

therefore β_{32}, β_{42} are given by:

$$\begin{pmatrix} \beta_2 & 0 \\ c_3 & c_4 \end{pmatrix} \begin{pmatrix} \beta_{32} \\ \beta_{42} \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix}$$

α_{32} can be calculated from (3.6): $\alpha_{32} = P_6(\gamma)/((c_3+c_4)\alpha_3\beta_2)$. β_4 follows from (3.2): $\beta_4 = (P_2(\gamma) - c_2\beta_2 - c_3\beta_3)/c_4$. ◆

The remaining free parameters, except γ, can be chosen so that several equations of condition of order five are satisfied. The coefficient γ determines essentially the stability properties, see (2.5), (2.6). c_4 has no influence on the truncation error, its value can be chosen to $c_3 = 0$.

Proposition (3.20). The free parameters of Proposition (3.19) are chosen as:

$$\alpha_2 = 2\gamma,$$

$$\alpha_3 = \frac{\frac{1}{5} - \frac{1}{4}\alpha_2}{\frac{1}{4} - \frac{1}{3}\alpha_2},$$

c_4 and β_{43} are solutions of the linear system:

$$\begin{pmatrix} \alpha_2^2 & \alpha_3^2 \\ \alpha_2^3 & \alpha_3^3 \end{pmatrix} \begin{pmatrix} c_2 & c_4\beta_{42} \\ c_4 & c_4\beta_{43} \end{pmatrix} = \begin{pmatrix} \frac{1}{3} & P_7(\gamma) \\ \frac{1}{4} & P_{14}(\gamma) \end{pmatrix}.$$

Then Eqs. (3.9), (3.10), (3.11), (3.14) and (3.15) are satisfied, too. It holds $c_3 = 0$.

Proof. For $\alpha_2 \neq \alpha_3$ the Eqs. (3.1), (3.3), (3.5) and (3.9) possess a solution, iff:

$$\det \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & \alpha_2^2 & \alpha_3^2 & \frac{1}{3} \\ 0 & \alpha_2^3 & \alpha_3^3 & \frac{1}{4} \\ 0 & \alpha_2^4 & \alpha_3^4 & \frac{1}{5} \end{pmatrix} = 0.$$

Thus the choice of α_3 implies (3.9). Due to the linear system it holds $c_3=0$ and (3.14). The choice of α_2 combined with (3.6) leads to the simplifying assumptions:

$$\sum_{k=1}^{s} \alpha_{ik}\beta_k=\alpha_i(\tfrac{1}{2}\alpha_i-\gamma).$$

Therefore (3.9) implies (3.10), (3.11). (3.14) implies (3.15), see also [13], Proposition 5, p. 20. ◆

Restriction. Evaluation of the righthand side of the differential equation merely in the integration interval requires:

$$0\leqq\alpha_i\leqq 1,\ i=2,\dots,s \qquad \text{(see [13, 14]).} \tag{3.21}$$

In order to obtain good values of γ, the E-polynomials (2.7) for a method (2.8) of order four and three are calculated. Because of the special structure of $R(z)$, see (2.4), it follows that $R(z)=e^z+O(z^{p+1})$

$$|P(z)|^2=|Q(z)|^2|e^z|^2+O(z^{p+1}). \tag{3.22}$$

For the imaginary axis $z=iy$, $y\in\mathbb{R}$, (3.22) reduces to polynomials of degree s in y^2. Since $|e^{iy}|=1$, the coefficients of y^{2k} $(0\leqq 2k\leqq p)$ are the same for $|P(iy)|^2$ and $|Q(iy)|^2$. Using (2.4) the E-polynomials can be calculated in a straightforward way.

Lemma (3.23). The E-polynomials (2.7) $\hat{E}$ of order 3 and E of order 4 are:

$$\hat{E}(y)=\hat{a}y^6+\hat{b}y^4,$$
$$E(y)=ay^8+by^6,$$

with

$$\hat{a}=\gamma^6\left(1-L_3\left(\frac{1}{\gamma}\right)^2\right)=-\frac{1}{36}+\frac{\gamma}{2}-\frac{13\gamma^2}{4}+\frac{28\gamma^3}{3}-12\gamma^4+6\gamma^5,$$
$$\hat{b}=\tfrac{1}{12}-\gamma+3\gamma^2-2\gamma^3,$$
$$a=\gamma^8\left(1-L_4\left(\frac{1}{\gamma}\right)^2\right)=-\frac{1}{576}+\frac{\gamma}{18}-\frac{25\gamma^2}{36}+\frac{13\gamma^3}{3}-\frac{173\gamma^4}{12}+\frac{76\gamma^5}{3}-22\gamma^6+8\gamma^7,$$
$$b=\frac{1}{72}-\frac{\gamma}{3}+\frac{17\gamma^2}{6}-\frac{32\gamma^3}{3}+17\gamma^4-8\gamma^5. \quad ◆$$

Applying (2.5) and (2.7) the method of order 4 is

A-stable, iff: $a\geqq 0$ and $b\geqq 0$,

stable at infinity, iff: $a\geqq 0$

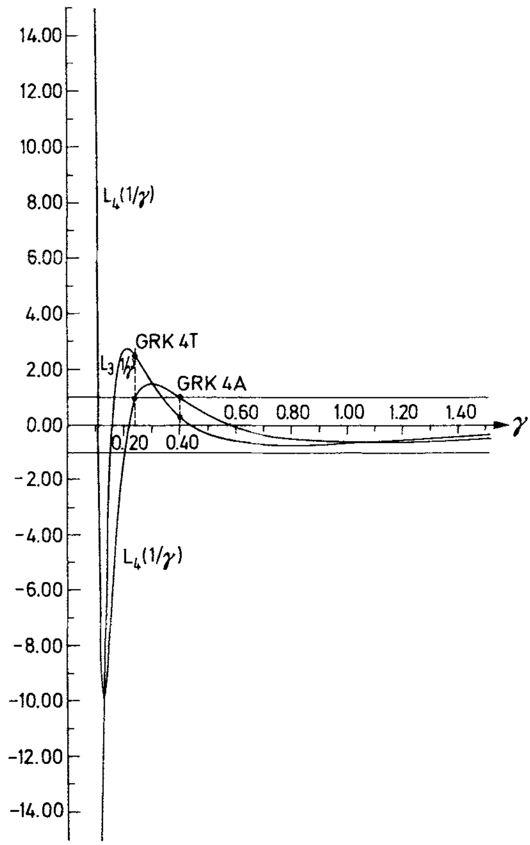
(analogue result for the method of order 3 with $\hat{a}, \hat{b}$). Computation of the zeros of a and b, resp. $\hat{a}$ and $\hat{b}$ leads to the stability intervals of γ, listed in Table (3.24).

Table (3.24). Stability Intervals

	A-stability	Stability at infinity, see also sketch (3.25)
$p=3$	$[\frac{1}{3}, 1.06858]$	$[0.15332, \frac{1}{6}] \cup [\frac{1}{3}, \infty[$
$p=4$	$[0.39434, 1.28057]$	$[0.10567, 0.10727] \cup [0.20385, 0.25] \cup [0.39434, \infty[$

The intervals of A-stability correspond to the recently published values of Burrage [4], Table 1.

Sketch (3.25). Laguerre Polynomials $L_3\left(\frac{1}{\gamma}\right)$, $L_4\left(\frac{1}{\gamma}\right)$



For the choice of γ, beside stability considerations the truncation error was taken into account. For a method of order p the local truncation error is given by:

$$h^{p+1} \sum_{i=1}^{N_{p+1}} T_i^{p+1} \alpha_i^{p+1} D_i^{p+1} + O(h^{p+2}), \qquad \text{see [3].}$$

The numerical constants T_i^{p+1} are determined by the parameters of the method, D_i^{p+1} are the elementary differentials of order $p+1$, α_i^{p+1} the corresponding coefficients of Butcher and N_{p+1} the number of trees of order $p+1$. The following expression defines the error constant:

$$\delta = \max |T_i^{p+1}| \tag{3.26}$$

Two methods with different γ and different stability properties are proposed. If both ROW-methods (2.8) should be A-stable, small values of γ lead to small truncation errors. Therefore $\gamma = 0.395$ is proposed. The hypotheses of Proposition (3.20) give $\alpha_3 < 0$, contradicting restriction (3.21). In Table (3.27) a coefficient set for $\gamma = 0.395$ with small truncation errors is listed, which don't satisfy (3.20).

Table (3.27). GRK4A, $\gamma = 0.395$

$\gamma = 0.395$	$\gamma_{21} = -0.767672395484$
$\gamma_{31} = -0.851675323742$	$\gamma_{32} = 0.522967289188$
$\gamma_{41} = 0.288463109545$	$\gamma_{42} = 0.880214273381E-1$
$\gamma_{43} = -0.337389840627$	
$\alpha_{21} = 0.438$	
$\alpha_{31} = 0.796920457938$	$\alpha_{32} = 0.730795420615E-1$
$\hat{c}_1 = 0.346325833758$	$\hat{c}_2 = 0.285693175712$
$\hat{c}_3 = 0.367980990530$	
$c_1 = 0.199293275701$	$c_2 = 0.482645235674$
$c_3 = 0.680614886256E-1$	$c_4 = 0.25$
$\delta \leq 0.942/5!$ for the method of order 4, see (3.26)	
$\hat{\delta} \leq 1.08/4!$ for the method of order 3, see (3.26)	

The second method is constructed according to Proposition (3.20). $\gamma \in [0.10567, 0.10727]$ produce great values of $L_3\left(\frac{1}{\gamma}\right)$. For $\gamma \in [0.20385, 0.25]$ $L_3\left(\frac{1}{\gamma}\right)$ is small, see sketch (3.25), and the stability region of the fourth order method is very large. For $\gamma = 0.231$ the fourth order method is $A(89.3°)$-stable, and the hypotheses of (3.20) and restriction (3.21) are satisfied. A coefficient set is listed in Table (3.28). A further related coefficient set with $\gamma = 0.22042841$ can be found in Stoer, Bulirsch [19].

Table (3.28). GRK4T, $\gamma = 0.231$

$\gamma = 0.231$	$\gamma_{21} = -0.270629667752$
$\gamma_{31} = 0.311254483294$	$\gamma_{32} = 0.852445628482E-2$
$\gamma_{41} = 0.282816832044$	$\gamma_{42} = -0.457959483281$
$\gamma_{43} = -0.111208333333$	
$\alpha_{21} = 0.462$	
$\alpha_{31} = -0.815668168327E-1$	$\alpha_{32} = 0.961775150166$
$\hat{c}_1 = -0.717088504499$	$\hat{c}_2 = 0.177617912176E+1$
$\hat{c}_3 = -0.590906172617E-1$	
$c_1 = 0.217487371653$	$c_2 = 0.486229037990$
$c_3 = 0.$	$c_4 = 0.296283590357$
$\delta \leq 0.199/5!$ for the method of order 4, see (3.26)	
$\hat{\delta} \leq 0.461/4!$ for the method of order 3, see (3.26)	

4. Numerical Implementation

To compute the vectors k_i (2.2), a linear system of order n for four right hand sides must be solved. In order to avoid matrix-vector multiplications, the equivalent form due to [21] is used:

$$
\begin{aligned}
&(I-h\gamma f'(y_0))\,k_1=hf(y_0),\\
&(I-h\gamma f'(y_0))(k_2+\tilde{\gamma}_{21}k_1)=hf(y_0+\alpha_{21}k_1)+\tilde{\gamma}_{21}k_1,\\
&(I-h\gamma f'(y_0))(k_3+(\tilde{\gamma}_{31}k_1+\tilde{\gamma}_{32}k_2))\\
&=hf(y_0+\alpha_{31}k_1+\alpha_{32}k_2)+(\tilde{\gamma}_{31}k_1+\tilde{\gamma}_{32}k_2),\\
&(I-h\gamma f'(y_0))(k_4+(\tilde{\gamma}_{41}k_1+\tilde{\gamma}_{42}k_2+\tilde{\gamma}_{43}k_3))\\
&=hf(y_0+\alpha_{31}k_1+\alpha_{32}k_2)+(\tilde{\gamma}_{41}k_1+\tilde{\gamma}_{42}k_2+\tilde{\gamma}_{43}k_3)
\end{aligned}
$$

where

$$\tilde{\gamma}_{ij}=\gamma_{ij}/\gamma.$$

The Jacobian $f'(y_0)$ is computed by difference approximation and should be replaced by an analytic version for very sensitive problems. The matrix $(I-h\gamma f'(y_0))$ is decomposed by LU-factorization. Computation of the k_i is equivalent to back substitutions. For large sparse systems the structure of the Jacobian is saved and the standard routine for LU-decomposition should be exchanged by subroutines for sparse systems. Both programs GRK4A (3.27) and GRK4T (3.28) have a structure as simple as the RKF methods [6, 7] and can be easily implemented. Except for generation of the Jacobian no nested loops are necessary. The calling sequence is in accordance with [6, 7].

5. Test Examples

The proposed methods were tested on 25 stiff differential equations [8]. The properties of the differential equations are only briefly described in the following, further informations can be found in [8]. The test set is divided into five classes:

Class A: Linear with real eigenvalues
Class B: Linear with non-real eigenvalues.
Class C: Nonlinear coupling with real eigenvalues.
Class D: Nonlinear with real eigenvalues.
Class E: Nonlinear with non-real eigenvalues.

The following abbreviations are used:

TZ: Total computing time in seconds to solve a problem. Computations were performed in FORTRAN single precision with a 38 bit mantissa (11 decimals) on the TR 440 of the Leibniz Rechenzentrum der Bayerischen Akademie der Wissenschaften.

FCN: Number of function calls

FJAC: Number of Jacobian evaluations. One evaluation of the Jacobian costs n function calls.

TF: Total number of function calls: TF = FCN + n-FJAC.

LU: Number of *LU*-decompositions, equivalent to the number of steps.

ERR: Maximum error of solution components at the end of the interval. The reference solution was computed by the procedure DRIVE with TOL = 1.E-8. DRIVE is the improved GEAR version from 13.1.1975, due to Gear [9] and Hindmarsh [12].

For all examples the initial stepsize $HI = 1.E-3$ and the stepsize control formula (2.9) were used. The test results are listed in Table (5.1) and Table (5.2).

Both methods solve all examples reliably. GRK4A looses precision in $D5$ and $E2$. According to precision and fastness, GRK4T is the superior method, in spite of its weaker stability conditions. Only in $E4$, the computing time of GRK4T is enlarged. An overall summary for both methods and for three tolerances in accordance with [8] is given in Table (5.3).

Table (5.1). Statistics for each problem, TOL = 1, $E-4$

Problem	GRK4A					
	TZ	LU	FCN	FJAC	TF	ERR
A1	0.31	40	120	40	280	$2.1E-7$
A2	1.22	53	155	49	596	$4.8E-8$
A3	0.44	60	175	55	395	$1.1E-6$
A4	2.01	74	213	65	863	$1.5E-6$
B1	1.44	183	542	176	1,246	$4.0E-5$
B2	0.49	40	120	40	360	$1.0E-6$
B3	0.53	43	129	43	387	$7.5E-7$
B4	0.77	62	186	62	558	$1.1E-6$
B5	2.04	164	492	164	1,476	$2.4E-6$
C1	0.36	45	135	45	315	$1.7E-7$
C2	0.37	43	129	43	301	$3.6E-7$
C3	0.45	53	159	53	371	$1.1E-5$
C4	1.04	122	366	122	854	$9.7E-6$
C5	1.32	154	462	154	2,919	$1.2E-5$
D1	1.19	207	621	207	1,242	$5.9E-6$
D2	0.46	78	231	75	456	$7.2E-5$
D3	0.38	49	140	42	308	$1.5E-7$
D4	0.14	25	75	25	150	$1.8E-5$
D5	0.11	28	84	28	140	$8.7E-3$
D6	0.13	23	69	23	138	$1.8E-4$
E1	1.81	288	552	184	1,288	$3.4E-10$
E2	0.33	87	250	76	402	$8.9E-4$
E3	0.48	80	238	78	472	$4.7E-5$
E4	0.79	78	229	73	521	$3.5E-4$
E5	0.26	33	99	33	231	$3.0E-8$

Table (5.2). Statistics for each probem, TOL $=1.E-4$

Problem	GRK4T					
	TZ	LU	FCN	FJAC	TF	ERR
A1	0.25	35	105	35	245	$1.6E-6$
A2	1.14	51	148	46	562	$2.1E-7$
A3	0.39	54	157	49	353	$2.0E-5$
A4	1.76	65	186	56	756	$2.0E-5$
B1	1.24	160	473	153	1,085	$3.6E-5$
B2	0.45	36	108	36	324	$1.2E-6$
B3	0.46	38	114	38	342	$1.6E-6$
B4	0.66	53	159	53	477	$2.0E-6$
B5	1.75	140	420	140	1,260	$1.7E-6$
C1	0.31	41	123	41	287	$1.8E-7$
C2	0.32	39	117	39	273	$5.0E-8$
C3	0.44	53	159	53	371	$1.5E-7$
C4	0.94	111	333	111	777	$1.2E-7$
C5	1.19	135	405	135	945	$4.5E-8$
D1	1.29	231	658	196	1,246	$3.8E-6$
D2	0.36	63	182	56	350	$4.9E-5$
D3	0.45	57	164	50	364	$3.2E-8$
D4	0.14	25	75	25	150	$2.2E-6$
D5	0.14	36	104	32	168	$1.1E-4$
D6	0.10	17	51	17	102	$2.9E-6$
E1	1.08	168	327	109	763	$3.4E-10$
E2	0.35	96	268	76	420	$4.6E-4$
E3	0.49	89	249	71	462	$4.3E-6$
E4	3.27	354	942	234	1,878	$9.7E-5$
E5	0.27	33	99	33	231	$3.3E-8$

Table (5.3). Overall Summary

Method	TOL	TZ	LU	FCN	FJAC	TF
GRK4A	$1.E-2$	9.39	1,066	2,851	927	6,859
	$1.E-4$	18.85	2,112	5,971	1,955	14,428
	$1.E-6$	65.35	7,271	21,189	7,088	49,324
GRK4T	$1.E-2$	8.40	960	2,666	864	6,419
	$1.E-4$	19.23	2,180	6,126	1,884	14,181
	$1.E-6$	58.07	6,676	19,179	6,320	43,336

Both methods are low order methods and work very well for low tolerances. They should be used only for tolerances between $1.E-2$ and $1.E-4$.

Comparison with DRIVE [9, 12]:

The improved GEAR version DRIVE is available to the authors. Computing time and function calls for all examples are listed in Table (5.4).

Table (5.4). Overall Summary for TOL $= 1.E-4$

		GRK4A	GRK4T	DRIVE-GEAR
All examples	TZ	18.85	19.23	44.21
	TF	14,428	14,181	9,099
All examples except B5, E4	TZ	16.02	14.21	21.57
	TF	12,431	11,043	5,423

Comparing computing time, both methods are competitive with DRIVE, although the number of function calls TF is enlarged by a factor two. DRIVE runs very efficient in the classes D and E, but produces heavy difficulties in B5, where precision is lost and computing time reaches 21.23 seconds. The great number of evaluations of the Jacobian and LU-decompositions in GRK4A and GRK4T are disadvantageous for large complicated systems, which are not included in the test set [8].

6. Application of GRK4A and GRK4T to the restricted Three Body Problem

To give some information how both methods will work for non-stiff differential equations, the restricted Three Body Problem (earth-moon-spaceship) tested in Bulirsch, Stoer [3] and [7] was solved. Results for the non-stiff differential equation solvers DIFSY1, VOAS, RKF7, and RKF4 from [6] together with GRK4A and GRK4T are listed in Table (6.1).

Table (6.1). Three Body Problem, TOL $= 1.E-4$, $HI = 1.E-3$

Statistics	DIFSY1	VOAS	RKF7	RKF4	GRK4A	GRK4T
TZ	1.11	2.36	1.28	1.44	1.89	2.48
TF	1,215	669	1,233	1,398	1,048	1,339

This difficult example, which requires a robust and reliable stepsize controll, was solved precisely by both methods. The more complicated structure of GRK4A and GRK4T enlarged the computing time by a factor 1.5, although the number of function calls is comparable to the related routine RKF4.

Conclusion

With GRK4A and GRK4T two reliable, fast and precise algorithms for the numerical solution of stiff systems of ordinary differential equations are available. The loworder methods should be applied for low tolerances up to TOL $= 1.E-4$. One would prefer these methods for problems with $n \lesssim 10$, because of the large number of LU-decompositions. If stability requirements are weaker GRK 4T seems to be the faster and more precise routine.

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