Conditions for the coefficients of Runge-Kutta methods for systems of n-th order differential equations

H.-M. Hebsaker (*)

ABSTRACT

To derive order conditions for Runge-Kutta methods of Nyström or Fehlberg type, applicable to arbitrary order differential equations, a theory similar to that about Runge-Kutta methods for first order systems, due to Butcher [1], is developed. By a new definition of elementary differentials, which is independent of the order of the given system, each condition to be satisfied by the coefficients of the method directly follows from the representation of the corresponding elementary differential.

1. INTRODUCTION

In the study of Runge-Kutta methods for the integration of systems of first order differential equations, Butcher [1] developed a calculus to expand both the solution and approximation vectors as Taylor series. A comparison of terms gives conditions on the parameters of the numerical process.
In consideration of the one-to-one correspondence of the elementary differentials (defined by Butcher) with rooted trees (see Kastlunger-Wanner [2], Hairer-Wanner [3,4]), several extensions of Butcher's theory were made to get more general integration methods. Especially the theory for Nyström methods to integrate second order systems, developed by Hairer [5] by the aid of first order partitioned systems, may be generalized to n-th order differential equations.
It is the aim of this paper to give a direct extension of Butcher's approach to systems of arbitrary order without using rooted trees. Giving a generalized definition for the elementary differentials, it is possible to state similar results as in [1], so that the order conditions for the coefficients of Runge-Kutta-Nyström methods can be derived immediately from the representations of the individual elementary differentials. This is applicable to Runge-Kutta algorithms of Nyström type [6,7,8] as well as to those of Fehlberg type [9]. To the latter method we give some applications at the end of this paper.
Let us consider a system of m coupled differential equations of n-th order

$$Y^{(n)} = F(x,y_1,y_1',\dots,y_1^{(n-1)},\dots,y_m,y_m',\dots,y_m^{(n-1)}),$$

$$= F(x,Y,Y',\dots,Y^{(n-1)}) \tag{1}$$

with the initial values $Y_0,Y_0',\dots,Y_0^{(n-1)}$ at the point x_0. The components of the vectors $Y^{(j)}$, $Y_0^{(j)}$ and F are denoted by $y_k^{(j)}$, $y_{k0}^{(j)}$ and f_k $(1\leqslant k\leqslant m,\ 0\leqslant j\leqslant n-1)$.

F is assumed to be sufficiently differentiable. To compute the approximation $Y_h^{(j)}$ of the solution $Y^{(j)}(x_0+h)$ (where h denotes the stepsize) the classical Runge-Kutta-Nyström method uses the formulas

$$Y_h^{(j)} = Y_0^{(j)} + h\,Y_0^{(j+1)} + \frac{h^2}{2!}\,Y_0^{(j+2)} + \dots$$

$$\dots + \frac{h^{n-j-1}}{(n-j-1)!}\,Y_0^{(n-1)} + h^{n-j}\sum_{\kappa=0}^{v} c_\kappa^{(n-j)}\,F_\kappa \quad (0\leqslant j\leqslant n-1) \tag{2}$$

with the evaluations

$F_0 = F(x_0,Y_0,Y_0',\dots,Y_0^{(n-1)})$ and

$$F_\kappa = F[x_0+\alpha_\kappa h,\ Y_0+\alpha_\kappa hY_0'+\dots+\frac{(\alpha_\kappa h)^{n-1}}{(n-1)!}Y_0^{(n-1)}$$

$$+h^n\sum_{\lambda=0}^{v}\beta_{\kappa\lambda}^{(n)}F_\lambda,$$

$$Y_0'+\alpha_\kappa hY_0''+\dots+\frac{(\alpha_\kappa h)^{n-2}}{(n-2)!}Y_0^{(n-1)}+h^{n-1}\sum_{\lambda=0}^{v}\beta_{\kappa\lambda}^{(n-1)}F_\lambda,$$

$$\vdots$$

$$Y_0^{(n-1)}+h\sum_{\lambda=0}^{v}\beta_{\kappa\lambda}^{(1)}F_\lambda]\ (1\leqslant\kappa\leqslant v). \tag{3}$$

To determine the coefficients $c_\kappa^{(n-j)}$, α_κ and $\beta_{\kappa\lambda}^{(n-j)}$ $(0\leqslant j\leqslant n-1;\ 0\leqslant\kappa,\lambda\leqslant v;\ \alpha_0=0)$ the Taylor series of $Y^{(j)}(x_0+h)$ and $Y_h^{(j)}$ at x_0 have to be compared.

2. THE TAYLOR EXPANSIONS FOR THE EXACT SOLUTION

The expansions of $Y^{(j)}(x_0+h)$ $(0\leqslant j\leqslant n-1)$ consist of

(*) Hans-Martin Hebsaker, Lehrstuhl für Mathematik I, Universität Gesamthochschule Siegen, Hölderlinstrasse 3, D-5900 SIEGEN 21, Federal Republic of Germany.

the initial values and the total derivatives $Y^{(n+k)}=F^{(k)}$ ($k\geqslant 0$) of (1), evaluated at x_0. To map the function

$$\varphi=\varphi(x,y_1,y_1',\dots,y_1^{(n-1)},\dots,y_m,y_m',\dots,y_m^{(n-1)}) \tag{4}$$

to its total derivative $\varphi'=\frac{d\varphi}{dx}$, the corresponding operator has the form

$$D=\frac{d}{dx}=d_x+\sum_{k=1}^{m}\sum_{j=0}^{n-1}y_k^{(j+1)}d_{kj} \tag{5}$$

(here, we denote $d_x=\partial/\partial x$, $d_{kj}=\partial/\partial y_k^{(j)}$ for $1\leqslant k\leqslant m$, $0\leqslant j\leqslant n-1$). By the expression

$$D^p(\varphi)=[d_x+\sum_{k=1}^{m}\sum_{j=0}^{n-1}y_k^{(j+1)}d_{kj}]^p(\varphi) \tag{6}$$

which was introduced by Collatz [10, p. 18] we get

$$D(\varphi+\psi)=D(\varphi)+D(\psi),\quad D(\varphi\cdot\psi)=D(\varphi)\cdot\psi+\varphi\cdot D(\psi),$$

$$D[D^p(\varphi)]=D^{p+1}(\varphi)+p\sum_{k=1}^{m}\sum_{j=0}^{n-2}y_k^{(j+2)}D^{p-1}[d_{kj}(\varphi)]$$

$$+p\sum_{k=1}^{m}D(f_k)\,D^{p-1}\,[d_{k(n-1)}(\varphi)]. \tag{7}$$

For $n=2$, these equations are identical to those of Bettis [6].

Definition 1

To simplify the successive derivation of (4) we define

$$E^0(\varphi)=\varphi,\ E^1(\varphi)=D(\varphi), \tag{8}$$

$$E^p(\varphi)=D^p(\varphi)+\sum_{r=1}^{[p/2]}A_r^p(\varphi)\ \text{with}$$

$$A_r^p(\varphi)=\frac{1}{r!}\sum_{k_1=1}^{m}\dots\sum_{k_r=1}^{m}\sum_{l_1=2}^{p}\sum_{l_2=2}^{l_1-2}\dots\sum_{l_r=2}^{l_{r-1}-2}\binom{p}{l_1}\binom{l_1}{l_2}\dots$$

$$\dots\binom{l_{r-1}}{l_r}\sum_{j_1=0}^{n-l_1+l_2}\dots\sum_{j_{r-1}=0}^{n-l_{r-1}+l_r}\sum_{j_r=0}^{n-l_r}y_{k_1}^{(j_1+l_1-l_2)}\dots$$

$$\dots y_{k_{r-1}}^{(j_{r-1}+l_{r-1}-l_r)}\,y_{k_r}^{(j_r+l_r)}\,D^{p-l_1}[d_{k_1j_1}\dots d_{k_rj_r}(\varphi)]$$

$$(p\geqslant 2,\ 1\leqslant r\leqslant[\tfrac{p}{2}]).$$

Here, $[\frac{p}{2}]$ denotes the greatest integer q such that $q\leqslant\frac{p}{2}$. For $i>k$ let $\sum_{j=i}^{k}(\dots)$ be zero.

In the case that $\varphi=F$ and $m=1$, Albrecht [11] already has considered the above expressions for $p\leqslant 3$.

Lemma 2

With the notation $d_{k(n-j)}=0$ for $j>n$ we obtain the new differentiation rule

$$D[E^p(\varphi)]=E^{p+1}(\varphi)+\sum_{\lambda=1}^{p}\binom{p}{\lambda}\sum_{k=1}^{m}E^1(f_k)E^{p-\lambda}(d_{k(n-\lambda)}(\varphi)). \tag{9}$$

Proof

By (7) and

$$\delta_0(\varphi)=\sum_{k_1=1}^{m}p\cdot\sum_{j_1=0}^{n-2}y_{k_1}^{(j_1+2)}D^{p-1}[d_{k_1j_1}(\varphi)],$$

$$\epsilon_0(\varphi)=\sum_{k=1}^{m}p.D(f_k)D^{p-1}[d_{k(n-1)}(\varphi)] \tag{10}$$

we get

$$D[D^p(\varphi)]=D^{p+1}(\varphi)+\delta_0(\varphi)+\epsilon_0(\varphi). \tag{11}$$

The expression

$$D[A_r^p(\varphi)]=\sum_{i=1}^{r}[\alpha_{r,i}(\varphi)+\beta_{r,i}(\varphi)]+\gamma_r(\varphi)+\delta_r(\varphi)+\epsilon_r(\varphi)$$

$$(1\leqslant r\leqslant[\tfrac{p}{2}]) \tag{12}$$

for the derivative of $A_r^p(\varphi)$ from (8) consists of terms which have similar expressions like $A_r^p(\varphi)$. Therefore we only describe these parts of them which differ from $A_r^p(\varphi)$:

$$\alpha_{r,i}(\varphi)=\frac{1}{r!}\sum_{k_1=1}^{m}\dots\sum_{j_1=0}^{n-l_i+l_{i+1}-1}\dots y_{k_i}^{(j_i+l_i-l_{i+1}+1)}\dots D^{p-l_1}[\dots(\varphi$$

$$\beta_{r,i}(\varphi)=\frac{1}{r!}\sum_{k_1=1}^{m}\dots\sum_{j_i=n-l_i+l_{i+1}}^{n-l_i+l_{i+1}}\dots D(f_{k_i})\dots D^{p-l_1}[\dots(\varphi)],$$

$$\gamma_r(\varphi)=\frac{1}{r!}\sum_{k_1=1}^{m}\dots D^{p+1-l_1}[\dots(\varphi)],\quad(1\leqslant i\leqslant r),$$

$$\delta_r(\varphi)=\frac{1}{r!}\sum_{k_1=1}^{m}\dots\sum_{k_{r+1}=1}^{m}\dots(p-l_1)\binom{p}{l_1}\dots\sum_{j_{r+1}=0}^{m-2}\dots$$

$$\dots y_{k_{r+1}}^{(j_{r+1}+2)}D^{p-1-l_1}[d_{k_1j_1}\dots d_{k_{r+1}j_{r+1}}(\varphi)],$$

$$\epsilon_r(\varphi)=\frac{1}{r!}\sum_{k=1}^{m}D(f_k)\sum_{k_1=1}^{m}\dots(p-l_1)\binom{p}{l_1}\dots$$

$$\dots D^{p-1-l_1}[d_{k_1j_1}\dots d_{k_rj_r}d_{k(n-1)}(\varphi)]\ . \tag{13}$$

After some special transformations (for the complete computation see [12]) we obtain

$$E^{p+1}(\varphi)=D^{p+1}(\varphi)+\sum_{r=1}^{[\frac{p+1}{2}]}A_r^{p+1}(\varphi)$$

$$=D^{p+1}(\varphi)+\delta_0(\varphi)+\sum_{r=1}^{[\frac{p}{2}]}[\sum_{i=1}^{r}\alpha_{r,i}(\varphi)+\gamma_r(\varphi)+\delta_r(\varphi)] \tag{14}$$

and

$$\sum_{\lambda=1}^{p}\binom{p}{\lambda}\sum_{k=1}^{m}E^1(f_k)\,E^{p-\lambda}[d_{k(n-\lambda)}(\varphi)]$$

$$= \epsilon_0(\varphi) + \sum_{r=1}^{[\frac{p}{2}]} [\sum_{i=1}^{r} \beta_{r,i}(\varphi) + \epsilon_r(\varphi)]. \tag{15}$$

From this equation (9) follows and lemma 2 is proved. Using equation (9) instead of the third rule of (7) the successive derivation of F from (1) may be considerably simplified. Furthermore it is possible to expand the theory by Butcher [1] immediately to systems of n-th order differential equations.

Definition 3

We denote

$$(p) = E^p(F) = \begin{bmatrix} E^p(f_1) \\ \cdot \\ \cdot \\ E^p(f_m) \end{bmatrix} \qquad (p \geq 0) \tag{16}$$

as an "elementary differential" of order p and degree s=0. The vector

$$G = \begin{bmatrix} g_1 \\ \cdot \\ \cdot \\ g_m \end{bmatrix} = (q|j_1,\dots,j_s)\, G_1 \dots G_s$$

$$= \sum_{k_1=1}^{m} \cdots \sum_{k_s=1}^{m} g_{1k_1} \cdots g_{sk_s} E^q[d_{k_1(n-j_1)} \cdots d_{k_s(n-j_s)}(F)] \tag{17}$$

with $q \geq 0$ and $1 \leq j_i \leq n$ $(1 \leq i \leq s)$ is called an elementary differential of degree $s \geq 1$ and order

$$u = q + \sum_{i=1}^{s} (j_i + u_i), \tag{18}$$

if g_{ik_i} $(1 \leq i \leq s)$ itself represents the k_i-th component of an elementary differential G_i of order $u_i \geq 1$.

Corollary 4

The order of every elementary differential of degree $s \geq 1$ is $u \geq 2$. The only elementary differentials of orders $u = 0$ and $u = 1$ are $F = (0)$ and $D(F) = (1)$.

Remark

The expressions j_i and G_i $(1 \leq i \leq s)$ are always coupled in G of (17). Therefore in general they cannot be changed separately with j_k or G_k without changing G by itself. If j_i and G_i are changed simultaneously with j_k and G_k, then G doesn't alter.

Notation

If some "pairs" (j_i, G_i) appear more than once in the expression (17) of G, then G is denoted by

$$G = (q|\underbrace{j_1,\dots,j_1}_{\mu_1\text{-fold}},\dots,\underbrace{j_\sigma,\dots,j_\sigma}_{\mu_\sigma\text{-fold}})\, G_1^{\mu_1} \dots G_\sigma^{\mu_\sigma}, \tag{19}$$

where μ_i $(1 \leq i \leq \sigma)$ denotes the multiplicity of (j_i, G_i) in G.

It holds $\sum_{i=1}^{\sigma} \mu_i = s$.

Example 5

$G = (0|1,1)(1)((1|2)(1))$ of the form (17) is equivalent to the expression

$$\sum_{k=1}^{m} \sum_{l=1}^{m} \sum_{r=1}^{m} E^1(f_r) E^1[d_{r(n-2)}(f_l)] E^1(f_k) E^0$$

$$[d_{l(n-1)}\, d_{k(n-1)}(F)].$$

It holds $q=0$, $s=\sigma=2$, $\mu_1=\mu_2=1$, $j_1=j_2=1$, $G_1=(1)$ and $G_2=(1|2)\,(1)$. The order of G_1 is $u_1=1$ by (16). Since G_2 is of the form (17), it holds $q_2=1$, $s_2=1$, $j_{21}=2$ and $G_{21}=(1)$ with $u_{21}=1$. Hence, with (18) it follows $u_2 = q_2 + (j_{21} + u_{21}) = 4$ and $u = q + (j_1 + u_1) + (j_2 + u_2) = 7$.

Remark

The order u of any given elementary differential G from (16) or (17) can be obtained by adding up all numbers which appear in the expression of G. In particular, the multiplicity in (19) has to be considered.

Corollary 6

The total derivatives of the elementary differentials (16) and (17) have the expressions

$$D[(p)] = (p+1) + \sum_{j_1=1}^{p} \binom{p}{j_1} (p-j_1|j_1)\,(1) \text{ and} \tag{20}$$

$$D[(q|j_1,\dots,j_s)G_1\dots G_s] = (q+1|j_1,\dots,j_s)G_1\dots G_s$$

$$+ \sum_{j_{s+1}=1}^{q} \binom{q}{j_{s+1}} (q-j_{s+1}|j_1,\dots,j_{s+1})\, G_1 \dots G_s \cdot (1)$$

$$+ \sum_{i=1}^{s} (q|j_1,\dots,j_s) G_1 \dots D[G_i] \dots G_s. \tag{21}$$

This follows from the use of (9).

Theorem 7

The total derivative of any elementary differential of order u consists of elementary differentials of order u+1. Their coefficients all are positive.

Proof

This results immediately by induction from corollaries 4 and 6 and equation (18).

Theorem 8

The p-th total derivative $F^{(p)}$ of F is a sum of elementary differentials of p-th order. There is no elementary differential of order p which does not appear in $F^{(p)}$.

Proof

The first assertion is obvious by corollary 4 and theorem 7. The proof of the existence of any elementary differential of p-th order in $F^{(p)}$ is done by induction. For $p \leqslant 1$ see corollary 4. If $p \geqslant 2$, we assume that the above assertion is true for $F^{(u)}$ $(1 \leqslant u \leqslant p-1)$. Let G be an arbitrary differential of order p. Then, by (20) and (21), one can find an elementary differential $\widetilde{G}$ of order p–1, so that G appears as a term in $D[\widetilde{G}]$ with some positive coefficient (see theorem 7). Since $\widetilde{G}$ is assumed to occur in $F^{(p-1)}$, G also must occur in $F^{(p)}$. Because the sum of positive coefficients is positive (G may occur more than once in $F^{(p)}$) the result is proved.

Example 9

By corollary 6 and theorems 7 and 8 the first derivatives of F are obtained as follows :

$$
\begin{aligned}
F' &= (1),\\
F'' &= (2) + (0\vert 1)(1), \qquad (22)\\
F''' &= (3) + (0\vert 1)(2) + 3(1\vert 1)(1) + (0\vert 1)^2(1) + (0\vert 2)(1).
\end{aligned}
$$

("$(0\vert 1)^2(1)$", "$(0\vert 1)(0\vert 1)(1)$" and "$(0\vert 1)((0\vert 1)(1))$" are notations for the same expression.)

Remark

The proofs of theorems 7 and 8 are similarly done as by Butcher (see theorems 1 and 2 in [1]). The more general definition of the elementary differentials enables us to use them for systems of n-th order differential equations too.
In table 1 all elementary differentials up to order 5 are presented in both the expressions by definition 3 and by Butcher. The coefficient a appearing in this table is explained later.

TABLE 1

Elementary differentials of orders 0-5 in the representations by definition 3 and by Butcher [1].

order u	el. diff. G by def. 3	G by Butcher	coeff. a
0	(0)	$\{1\}$	1
1	(1)	$\{f\}$	1
2	(2)	$\{f^2\}$	1
	$(0\vert 1)(1)$	$\{_2 f\}_2$	1
3	(3)	$\{f^3\}$	1
	$(0\vert 1)(2)$	$\{_2 f^2\}_2$	1
	$(1\vert 1)(1)$	$\{f\{f\}\}$	3
	$(0\vert 1)^2(1)$	$\{_3 f\}_3$	1
	$(0\vert 2)(1)$	———	1
4	(4)	$\{f^4\}$	1
	$(0\vert 1)(3)$	$\{_2 f^3\}_2$	1
	$(1\vert 1)(2)$	$\{f\{f^2\}\}$	4
	$(2\vert 1)(1)$	$\{f^2\{f\}\}$	6
	$(0\vert 1)^2(2)$	$\{_3 f^2\}_3$	1
	$(0\vert 1)(1\vert 1)(1)$	$\{_2 f\{f\}\}_2$	3
	$(1\vert 1)(0\vert 1)(1)$	$\{f\{_2 f\}_2\}$	4
	$(0\vert 1)^3(1)$	$\{_4 f\}_4$	1
	$(0\vert 1,1)(1)^2$	$\{\{f\}^2\}$	3
	$(0\vert 2)(2)$	———	1
	$(1\vert 2)(1)$	———	4
	$(0\vert 2)(0\vert 1)(1)$	———	1
	$(0\vert 1)(0\vert 2)(1)$	———	1
	$(0\vert 3)(1)$	———	1
5	(5)	$\{f^5\}$	1
	$(0\vert 1)(4)$	$\{_2 f^4\}_2$	1
	$(1\vert 1)(3)$	$\{f\{f^3\}\}$	5
	$(2\vert 1)(2)$	$\{f^2\{f^2\}\}$	10
	$(3\vert 1)(1)$	$\{f^3\{f\}\}$	10
	$(0\vert 1)^2(3)$	$\{_3 f^3\}_3$	1
	$(0\vert 1)(1\vert 1)(2)$	$\{_2 f\{f^2\}\}_2$	4
	$(0\vert 1)(2\vert 1)(1)$	$\{_2 f^2\{f\}\}_2$	6
	$(1\vert 1)(0\vert 1)(2)$	$\{f\{_2 f^2\}_2\}$	5
	$(1\vert 1)^2(1)$	$\{f\{f\{f\}\}\}$	15
	$(2\vert 1)(0\vert 1)(1)$	$\{f^2\{_2 f\}_2\}$	10
	$(0\vert 1)^3(2)$	$\{_4 f^2\}_4$	1
	$(0\vert 1)^2(1\vert 1)(1)$	$\{_3 f\{f\}\}_3$	3
	$(0\vert 1)(1\vert 1)(0\vert 1)(1)$	$\{_2 f\{_2 f\}_2\}_2$	4
	$(1\vert 1)(0\vert 1)^2(1)$	$\{f\{_3 f\}_3\}$	5
	$(0\vert 1)^4(1)$	$\{_5 f\}_5$	1
	$(0\vert 1,1)(1)(2)$	$\{\{f\}\{f^2\}\}$	10
	$(1\vert 1,1)(1)^2$	$\{f\{f\}^2\}$	15
	$(0\vert 1,1)(1)((0\vert 1)(1))$	$\{\{f\}\{_2 f\}_2\}$	10
	$(0\vert 1)(0\vert 1,1)(1)^2$	$\{_2\{f\}^2\}_2$	3

order u	el. diff. G by def. 3	G by Butcher	coeff. a
5	(0|2)(3)	———	1
	(1|2)(2)	———	5
	(2|2)(1)	———	10
	(0|1)(0|2)(2)	———	1
	(0|1)(1|2)(1)	———	4
	(1|1)(0|2)(1)	———	5
	(0|2)(0|1)(2)	———	1
	(0|2)(1|1)(1)	———	3
	(1|2)(0|1)(1)	———	5
	$(0\|2)^2(1)$	———	1
	$(0\|1)^2(0\|2)(1)$	———	1
	(0|1)(0|2)(0|1)(1)	———	1
	$(0\|2)(0\|1)^2(1)$	———	1
	$(0\|1,2)(1)^2$	———	10
	(0|3)(2)	———	1
	(1|3)(1)	———	5
	(0|1)(0|3)(1)	———	1
	(0|3)(0|1)(1)	———	1
	(0|4)(1)	———	1

The existence of all elementary differentials in the total derivatives of F now is proved. To construct the Taylor expansion

$$Y^{(j)}(x_0+h)$$

$$= Y_0^{(j)} + h\,Y_0^{(j+1)} + \ldots + \frac{h^{n-j}}{(n-j)!}\,F_0 + \sum_{p=1}^{\infty} \frac{h^{n-j+p}}{(n-j+p)!}\,F^{(p)}(x_0,\ldots,Y_0^{(n-1)})$$

$$= Y_0^{(j)} + h\,Y_0^{(j+1)} + \ldots + \frac{h^{n-j}}{(n-j)!}\,F_0 + \sum_{i=1}^{\infty} \frac{h^{n-j+u_i}}{(n-j+u_i)!}\,a_i\,(G_i)_0 \qquad (0 \leqslant j \leqslant n-1), \tag{23}$$

where all elementary differentials of order $u \geqslant 1$ are numbered throughout $((\ldots)_0$ designates the evaluation of the expression at $(x_0, Y_0, Y_0', \ldots, Y_0^{(n-1)}))$, the coefficients a_i of G_i have still be found. The application of corollary 6 to find the coefficient a_i where G_i is an elementary differential of high order, becomes increasingly involved. Therefore we will prove a formula to compute a_i only from the corresponding elementary differential G_i. However let us prove at first a lemma which will also be used in the computation of the Taylor series of $Y_h^{(j)}$ $(0 \leqslant j \leqslant n-1)$.

Notation

If we define the vector H_l with the components η_{kl} $(1 \leqslant k \leqslant m)$ as

$$H_l = l!\,.\sum_{p=1}^{\infty} \frac{h^p}{(l+p)!}\,F^{(p)} \qquad (1 \leqslant l \leqslant n), \tag{24}$$

then the Taylor expansion of $y_k^{(j)}(x+h)$ $(1 \leqslant k \leqslant m,$ $0 \leqslant j \leqslant n-1)$ at x takes the form

$$y_k^{(j)}(x+h)$$

$$= y_k^{(j)} + h\,y_k^{(j+1)} + \ldots + \frac{h^{n-j}}{(n-j)!}\,f_k + \sum_{p=1}^{\infty} \frac{h^{n-j+p}}{(n-j+p)!}\,f_k^{(p)}$$

$$= y_k^{(j)} + h\,y_k^{(j+1)} + \ldots + \frac{h^{n-j}}{(n-j)!}\,f_k + \frac{h^{n-j}}{(n-j)!}\,\eta_{k(n-j)}. \tag{25}$$

Lemma 10

Let φ from (4) be analytical in some neighborhood of $(x, y_1(x), \ldots, y_m^{(n-1)}(x))$. Consider the point $(x+ch, \tilde{y}_1, \ldots, \tilde{y}_m^{(n-1)})$ within this neighborhood, where $\tilde{y}_k^{(j)}$ $(1 \leqslant k \leqslant m,\ 0 \leqslant j \leqslant n-1)$ is defined as

$$\tilde{y}_k^{(j)} = y_k^{(j)} + ch\,y_k^{(j+1)} + \ldots + \frac{(ch)^{n-j}}{(n-j)!}\,f_k + \frac{h^{n-j}}{(n-j)!}\,\eta_{k(n-j)} \tag{26}$$

with sufficiently small h. Then the Taylor series of

$$\varphi_h = \varphi(x+ch, \tilde{y}_1, \ldots, \tilde{y}_m^{(n-1)}) \tag{27}$$

at $(x, y_1(x), \ldots, y_m^{(n-1)}(x))$ admits the form

$$\varphi_h = \varphi + \sum_{p=1}^{\infty} \frac{h^p}{p!}\,\Big\{c^p E^p(\varphi) + \sum_{r=1}^{p} \frac{1}{r!} \sum_{l_1=r}^{p} \sum_{l_2=r-1}^{l_1-1} \cdots$$

$$\cdots \sum_{l_r=1}^{l_{r-1}-1} c^{p-l_1} \binom{p}{l_1}\binom{l_1}{l_2}\cdots\binom{l_{r-1}}{l_r} \sum_{k_1=1}^{m} \cdots \sum_{k_r=1}^{m} \eta_{k_1(l_1-l_2)} \cdot$$

$$\cdots \eta_{k_{r-1}(l_{r-1}-l_r)}\,\eta_{k_r l_r}\,E^{p-l_1}\,[d_{k_1(n-l_1+l_2)} \cdots$$

$$\cdots d_{k_{r-1}(n-l_{r-1}+l_r)}\,d_{k_r(n-l_r)}(\varphi)]\Big\}. \tag{28}$$

Proof

Observe that the Taylor expansion of φ_h at $(x, y_1(x), \ldots, y_m^{(n-1)}(x))$ has the form

$$\varphi_h = \varphi + \sum_{p=1}^{\infty} \frac{1}{p!}\Big(ch\,d_x + \sum_{k=1}^{m} \sum_{j=0}^{n-1} \sum_{l=1}^{n-j} \frac{(ch)^l}{l!}\,y_k^{(j+l)} d_{kj}$$

$$+\sum_{k=1}^{m}\sum_{j=0}^{n-1}\frac{h^{n-j}}{(n-j)!}\eta_{k(n-j)}\,d_{kj})^{p}(\varphi)$$

$$=\varphi+\sum_{p=1}^{\infty}\frac{1}{p!}(ch\,D+\sum_{k=1}^{m}\sum_{l=2}^{n}\frac{(ch)^{l}}{l!}\sum_{j=0}^{n-1}y_k^{(j+l)}\,d_{kj}$$

$$+\sum_{k=1}^{m}\sum_{l=1}^{n}\frac{h^{l}}{l!}\eta_{kl}\,d_{k(n-l)})^{p}(\varphi). \qquad (29)$$

For computing the second expression of (29) we use the notations $\sum_{j=i}^{k}(\dots)=0$ for $i>k$ and $d_{k(n-j)}=0$ for $j>n$ as in definition 1 and lemma 2. Those terms of the resulting expression are combined, which include the same powers of h as a factor. Using definition 1 we obtain equation (28), and the lemma is proved (for details see [12]).

Corollary 11

If we replace φ by F and set $c=1$ in lemma 10, then

$$F_h=F[x+h,y_1(x+h),\dots,y_m^{(n-1)}(x+h)] \qquad (30)$$

has the following Taylor expansion at $(x,y_1(x),\dots,y_m^{(n-1)}(x))$, using definition 3 :

$$F_h=F+\sum_{p=1}^{\infty}\frac{h^p}{p!}[(p)+\sum_{r=1}^{p}\frac{1}{r!}\sum_{l_1=r}^{p}\sum_{l_2=r-1}^{l_1-1}\cdots\sum_{l_r=1}^{l_{r-1}-1}\cdots$$

$$\cdots\frac{p!}{(p-l_1)!(l_1-l_2)!\dots(l_{r-1}-l_r)!l_r!}\cdots$$

$$\cdots(p-l_1|l_1-l_2,\dots,l_{r-1}-l_r,l_r)H_{l_1-l_2}\cdots H_{l_{r-1}-l_r}H_{l_r}]. \qquad (31)$$

Thus we get the following result for the coefficients a_i in (23) :

Theorem 12

Let $G=(q|\underbrace{j_1,\dots,j_1}_{\mu_1\text{-fold}},\dots,\underbrace{j_\sigma,\dots,j_\sigma}_{\mu_\sigma\text{-fold}})\,G_1^{\mu_1}\dots G_\sigma^{\mu_\sigma}$ be an arbitrary elementary differential of order u and degree $s=\sum_{i=1}^{\sigma}\mu_i\geq 1$. Let a denote the coefficient of G in the expression (23), so that a.G is a term of the u-th derivative of F. Simultaneously the variables a_i may denote the corresponding coefficients of the elementary differentials G_i of order u_i $(1\leq i\leq\sigma)$ which appear as some "factors" in G. Then a is recursively determined by

$$a=\frac{u!}{q!}\cdot\prod_{i=1}^{\sigma}\frac{1}{\mu_i!}\left(\frac{a_i}{(j_i+u_i)!}\right)^{\mu_i}. \qquad (32)$$

Proof

If G_i $(i=1,2,3,\dots)$ are all elementary differentials of orders $u_i\geq 1$, which all occur in the total derivatives $F^{(p)}$ $(p\geq 1)$ by theorem 8, then the Taylor series of $F_h=Y^{(n)}(x+h)$ at x may be described as follows :

$$F_h=F+\sum_{p=1}^{\infty}\frac{h^p}{p!}F^{(p)}=(0)+\sum_{i=1}^{\infty}\frac{h^{u_i}}{u_i!}a_iG_i. \qquad (33)$$

On the other hand this is identical with (31). Therefore a can be found by equating (31) and (33). If G of degree s contains exactly τ distinct values j_k and to each j_k $(1\leq k\leq\tau)$ exactly σ_k distinct elementary differentials G_{ki} $(1\leq i\leq\sigma_k)$, so that the pairs (j_k,G_{ki}) appear in G with multiplicity ρ_{ki}, then G may be described in the form

$$G=(q|\underbrace{j_1,\dots,j_1}_{\nu_1\text{-fold}},\dots,\underbrace{j_\tau,\dots,j_\tau}_{\nu_\tau\text{-fold}})G_1\dots G_{\nu_1}\dots G_s$$

$$=(q|\underbrace{j_{11},\dots,j_{11}}_{\rho_{11}\text{-fold}},\dots,\underbrace{j_{1\sigma_1},\dots,j_{1\sigma_1}}_{\rho_{1\sigma_1}\text{-fold}},\dots,\underbrace{j_{\tau\sigma_\tau},\dots,j_{\tau\sigma_\tau}}_{\rho_{\tau\sigma_\tau}\text{-fold}})G_{11}^{\rho_{11}}\dots$$

$$\dots G_{1\sigma_1}^{\rho_{1\sigma_1}}\dots G_{\tau\sigma_\tau}^{\rho_{\tau\sigma_\tau}} \qquad (34)$$

with $j_{ki}=j_k$, $\sum_{i=1}^{\sigma_k}\rho_{ki}=\nu_k$ $(1\leq k\leq\tau,\ 1\leq i\leq\sigma_k)$, $\sum_{k=1}^{\tau}\nu_k=s$. G from (34) occurs only in those terms of (31) where $r=s$, $p-l_1=q$ and $l_1=\sum_{i=1}^{s}j_i$ holds. Furthermore the sets $\{j_1,\dots,j_s\}$ and $\{l_1-l_2,\dots,l_{s-1}-l_s,l_s\}$ must be equal. Since any permutations of the pairs (j_i,G_i) in (34) are permissible (see the remark after corollary 4), there are $\left(\frac{s!}{\nu_1!\dots\nu_\tau!}\right)$ possibilities to equate $(q|j_1,\dots,j_s)$ and $(q|l_1-l_2,\dots,l_s)$. Hence, all terms of (31) which include G occur in

$$\frac{h^p}{q!}\cdot\prod_{k=1}^{\tau}\left(\frac{1}{\nu_k!(j_k!)^{\nu_k}}\right)(q|\underbrace{j_1,\dots,j_1}_{\nu_1\text{-fold}},\dots,\underbrace{j_\tau,\dots,j_\tau}_{\nu_\tau\text{-fold}})H_{j_1}^{\nu_1}\dots H_{j_\tau}^{\nu_\tau} \qquad (35)$$

with $p=q+\sum_{k=1}^{\tau}\nu_kj_k$. Now, for some k $(1\leq k\leq\tau)$, we consider those elementary differentials G_i in G which are coupled with j_k. With their multiplicity they are represented exactly $\left(\frac{\nu_k!}{\rho_{k1}!\dots\rho_{k\sigma_k}!}\right)$ times in

$$H_{j_k}^{\nu_k}=(j_k!)^{\nu_k}\cdot\left[\sum_{i=1}^{\infty}\frac{h^{u_i}}{(j_k+u_i)!}a_i\,G_i\right]^{\nu_k} \qquad (36)$$

(see (24) and (33)). Therefore (with $j_{ki}=j_k$ $(1\leq k\leq\tau$, $1\leq i\leq\sigma_k))$

$$\frac{h^p}{q!}\cdot\prod_{k=1}^{\tau}\prod_{i=1}^{\sigma_k}\frac{1}{\rho_{ki}!}\left[\frac{h^{u_{ki}}a_{ki}}{(j_{ki}+u_{ki})!}\right]^{\rho_{ki}} \qquad (37)$$

$$\cdot(q|\underbrace{j_{11},\ldots,j_{11}}_{\rho_{11}\text{-fold}},\ldots,\underbrace{j_{\tau\sigma_\tau},\ldots,j_{\tau\sigma_\tau}}_{\rho_{\tau\sigma_\tau}\text{-fold}})\,G_{11}^{\rho_{11}}\ldots G_{\tau\sigma_\tau}^{\rho_{\tau\sigma_\tau}}$$

is precisely that term of (31) which includes the considered elementary differential G of (34). By designating the terms $j_{11},\ldots,j_{\tau\sigma_\tau}$, $\rho_{11},\ldots,\rho_{\tau\sigma_\tau}$ to $j_1,\ldots,j_\sigma$, $\mu_1,\ldots,\mu_\sigma$ ($\sigma=\sum_{k=1}^{\tau}\sigma_k$) we finally get the equation

$$\frac{h^u}{u!}\,a\,G=\frac{h^p}{q!}\cdot\prod_{i=1}^{\sigma}\frac{1}{\mu_i!}\left(\frac{h^{u_i}a_i}{(j_i+u_i)!}\right)^{\mu_i}$$

$$\cdot(q|\underbrace{j_1,\ldots,j_1}_{\mu_1\text{-fold}},\ldots,\underbrace{j_\sigma,\ldots,j_\sigma}_{\mu_\sigma\text{-fold}})\,G_1^{\mu_1}\ldots G_\sigma^{\mu_\sigma} \tag{38}$$

with $p+\sum_{i=1}^{\sigma}\mu_i u_i=q+\sum_{i=1}^{\sigma}\mu_i(j_i+u_i)=u$ by (18).
From this however the result of theorem 12 follows.

Remark

If G is an elementary differential of degree s=0, then a=1. This follows by $F'=(1)$ and equation (20). The coefficients a of all elementary differentials of orders $u\leqslant 5$ are presented in table 1.

Now, the Taylor expansions of $Y^{(j)}(x_0+h)$ at x_0 ($0\leqslant j\leqslant n-1$) are representable explicitly by the elementary differentials of definition 3. This is generally true and not restricted to Runge-Kutta methods.

3. THE TAYLOR SERIES FOR THE APPROXIMATION

To construct the conditions for the Runge-Kutta coefficients the Taylor expansions of the approximations $Y_h^{(j)}$ ($0\leqslant j\leqslant n-1$) additionally are requested. In particular, these approximations consist of the function evaluations F_κ ($1\leqslant\kappa\leqslant v$, see (2)). Therefore the expansions of $Y_h^{(j)}$ at x_0 can be obtained by constructing the Taylor series of F_κ at $(x_0,Y_0,Y_0',\ldots,Y_0^{(n-1)})$. Considering the arguments

$$Y_0^{(j)}+\alpha_\kappa h\,Y_0^{(j+1)}+\ldots+\frac{(\alpha_\kappa h)^{n-j-1}}{(n-j-1)!}\,Y_0^{(n-1)}$$

$$+h^{n-j}\sum_{\lambda=0}^{v}\beta_{\kappa\lambda}^{(n-j)}F_\lambda \tag{39}$$

($0\leqslant j\leqslant n-1$) of F_κ from (3) as Taylor series, we obtain the usual but not necessary conditions

$$\sum_{\lambda=0}^{v}\beta_{\kappa\lambda}^{(n-j)}=\frac{\alpha_\kappa^{n-j}}{(n-j)!}\qquad(0\leqslant j\leqslant n-1,\ 1\leqslant\kappa\leqslant v), \tag{40}$$

which simplify the construction of the Runge-Kutta conditions (see also Hairer-Wanner [7]).

Definition 13

Using (40) we define for $1\leqslant\kappa\leqslant v$:

$$R_\kappa=F_\kappa-F_0$$

$$=F(x_0+\alpha_\kappa h,\ Y_0+\alpha_\kappa h\,Y_0'+\ldots+\frac{(\alpha_\kappa h)^n}{n!}F_0+h^n\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(n)}R_\lambda,$$

$$Y_0'+\alpha_\kappa h\,Y_0''+\ldots+\frac{(\alpha_\kappa h)^{n-1}}{(n-1)!}F_0+h^{n-1}\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(n-1)}R_\lambda,$$

$$\vdots$$

$$Y_0^{(n-1)}+h\,F_0+h\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(1)}R_\lambda)-F_0. \tag{41}$$

Corollary 14

The vector R_κ ($1\leqslant\kappa\leqslant v$) from (41) can be represented by

$$R_\kappa=\sum_{p=1}^{\infty}h^p\Big[\frac{\alpha_\kappa^p}{p!}(p)_0+\sum_{r=1}^{p}\frac{1}{r!}\sum_{l_1=r}^{p}\sum_{l_2=r-1}^{l_1-1}\ldots$$

$$\ldots\sum_{l_r=1}^{l_{r-1}-1}\frac{\alpha_\kappa^{p-l_1}}{(p-l_1)!}\,(p-l_1|l_1-l_2,\ldots,l_{r-1}-l_r,l_r)_0$$

$$\cdot\Big(\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(l_1-l_2)}R_\lambda\Big)\ldots\Big(\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(l_{r-1}-l_r)}R_\lambda\Big)\Big(\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(l_r)}R_\lambda\Big)\Big]. \tag{42}$$

This follows immediately from lemma 10 and corollary 11 by replacing $\frac{1}{l!}H_l$ by $(\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(l)}R_\lambda)$ ($1\leqslant l\leqslant n$) and setting $c=\alpha_\kappa$.

Corollary 15

Assuming (40), F_κ from (3) is a sum of elementary differentials, evaluated at x_0. Hence, we obtain the expression

$$F_\kappa=F_0+\sum_{i=1}^{\infty}h^{u_i}b_{\kappa i}(G_i)_0\qquad(1\leqslant\kappa\leqslant v) \tag{43}$$

with some coefficients $b_{\kappa i}$ and some powers u_i. This follows by inserting successively the expression (42) into itself.

Theorem 16

For any elementary differential G which occurs in R_κ ($1\leqslant\kappa\leqslant v$) from (42), the corresponding term has the form $h^u b_\kappa G_0$ ($G_0=G|_{x=x_0}$). The exponent u of h is exactly the order of G. If G = (p), then

$$b_\kappa=\frac{\alpha_\kappa^p}{p!}. \tag{44}$$

If $G = (q|\underbrace{j_1,\dots,j_1}_{\mu_1\text{-fold}},\dots,\underbrace{j_\sigma,\dots,j_\sigma}_{\mu_\sigma\text{-fold}})\, G_1^{\mu_1}\dots G_\sigma^{\mu_\sigma}$ has the degree $s=\sum_{i=1}^{\sigma}\mu_i \geq 1$, then b_κ can be recursively computed by

$$b_\kappa = \frac{a_\kappa^q}{q!}\cdot\prod_{i=1}^{\sigma}\frac{1}{\mu_i!}\Big(\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(j_i)}\, b_{\lambda i}\Big)^{\mu_i}. \qquad (45)$$

Here, $b_{\lambda i}$ ($1\leq i\leq\sigma$, $1\leq\lambda\leq v$) are the corresponding coefficients of G_i in R_λ.

Proof

In the case $G=(p)$ the result follows directly from the representation of R_κ in (42). The construction of equation (45) is similar to the proof of (32) in theorem 12. Therefore we only describe that therm of R_κ which includes the elementary differential $G = (q|j_1,\dots,j_1,\dots,j_\sigma,\dots,j_\sigma)\, G_1^{\mu_1}\dots G_\sigma^{\mu_\sigma}$ as the only one :

$$h^u b_\kappa G_0 = \frac{a_\kappa^q}{q!}\cdot(q|\underbrace{j_1,\dots,j_1}_{\mu_1\text{-fold}},\dots,\underbrace{j_\sigma,\dots,j_\sigma}_{\mu_\sigma\text{-fold}})_0$$

$$\cdot\, h^{p+\mu_1 u_1+\dots+\mu_\sigma u_\sigma}\cdot\prod_{i=1}^{\sigma}\frac{1}{\mu_i!}\Big[\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(j_i)}\, b_{\lambda i}(G_i)_0\Big]^{\mu_i}. \qquad (46)$$

If we assume that u_i ($1\leq i\leq\sigma$) is the order of G_i, then, by induction, the exponent u of h is exactly the order of G. This follows by $p = q+\sum_{i=1}^{\sigma}\mu_i j_i$ and (18).

Example 17

To illustrate the formulas (32) and (45) we determine the condition of the Runge-Kutta coefficients which is generated by the elementary differential $G = (0|1,1)(1)((1|2)(1))$ of example 5. For $G_1=G_{21}=(1)$ it holds $a_1=a_{21}=1$ and $b_{\kappa 1}=b_{\kappa 21}=\alpha_\kappa$ ($1\leq\kappa\leq v$). For $G_2 = (1|2)(1)$ it follows

$$a_2 = \frac{4!.1}{1!.(2+1)!} = 4,\quad b_{\kappa 2} = \frac{\alpha_\kappa}{1!}\cdot\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(2)}\alpha_\lambda. \qquad (47)$$

The coefficients a and b_κ ($1\leq\kappa\leq v$) finally are computed as

$$a = \frac{7!.1.4}{0!.(1+1)!.(4+1)!} = \frac{7!.4}{2!.5!} = 84 \text{ and}$$

$$b_\kappa = \frac{\alpha_\kappa^0}{0!}\cdot\Big(\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(1)}\alpha_\lambda\Big)\Big(\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(1)}\alpha_\lambda\sum_{\mu=1}^{v}\beta_{\lambda\mu}^{(2)}\alpha_\mu\Big). \qquad (48)$$

Comparing the Taylor expansions of $Y^{(j)}(x_0+h)$ and $Y_h^{(j)}$ at x_0 ($0\leq j\leq n-1$, see (23) and (2)) the condition for the Runge-Kutta coefficients, generated by $G = (0|1,1)(1)((1|2)(1))$ admits the representation

$$\frac{84}{(n-j+7)!} = \sum_{\kappa=1}^{v} c_\kappa^{(n-j)}\Big(\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(1)}\alpha_\lambda\Big)\Big(\sum_{\lambda=1}^{v}\beta_{\kappa\lambda}^{(1)}\alpha_\lambda\sum_{\mu=1}^{v}\beta_{\lambda\mu}^{(2)}\alpha_\mu\Big). \qquad (49)$$

4. COMPARING THE PRECEDING RESULTS WITH A THEORY FOR NYSTRÖM METHODS, BASED ON PARTITIONED ORDINARY DIFFERENTIAL EQUATIONS

Interpreting x as a dependent variable with $x' \equiv 1$, $x^{(j)} \equiv 0$ ($2\leq j\leq n-1$), the system (1) may be considered as a partitioned system of first order differential equations of the form

$$Y_j' = \tilde{F}_j(Y_1,\dots,Y_n) \qquad (1\leq j\leq n), \qquad (50)$$

where $Y^{(j-1)}$ is replaced by Y_j and

$$\tilde{F}_j(Y_1,\dots,Y_n) = Y_{j+1} \qquad (1\leq j\leq n-1),$$
$$\tilde{F}_n(Y_1,\dots,Y_n) = F(Y_1,\dots,Y_n) \qquad (51)$$

holds from (1), including x to the vector Y_1. Using P-series for representing the solution and approximation of (50) as Taylor series at x_0 (see Hairer [5]), the order conditions for the Runge-Kutta coefficients follow from the study of the set TN of special P-trees, defined in [5].

Assuming (40), the remaining subset of TN can easily be found by using definition 2 : Let t_G denote the rooted tree corresponding to the elementary differential G (an explanation of rooted trees is given in [2,3,7]). Then $t_{(p)}$ consists of one fat node called the root of $t_{(p)}$ with index n, and p meagre end-nodes above without some index, which are connected with the root each by one arc. (The indices of P-trees should not be mixed up with the monotonic labelling of trees, which is not considered here). If $G = (q|j_1,\dots,j_s)G_1\dots G_s$ as defined in (17), t_G is got as follows : connect the roots of t_{G_i} ($1\leq i\leq s$) with a new fat node (the root of t_G with index n) along some lines consisting of j_i arcs and j_i-1 meagre nodes, which are labelled by $n-j_i+1$, $n-j_i+2,\dots,n-1$. Furthermore put q arcs with meagre end-nodes to the root of t_G (see the fourth tree of Fig. 1).

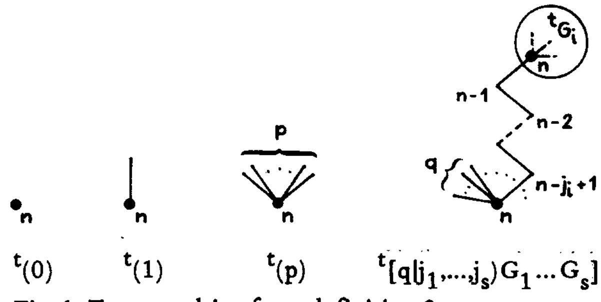
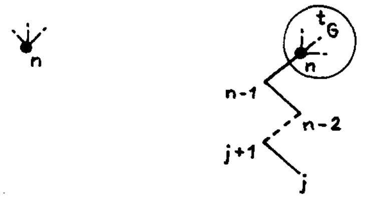


Fig. 1. Trees resulting from definition 2.

The total number of arcs occuring in t_G is identical with the order u of G. The rules of corollary 6 are interpreted as follows :

1. Put an arc with a meagre end-node to each fat node.
2. If q end-nodes are connected with one fat node as seen in fig. 1, then for all $j \in \{1,...,q\}$, replace j end-nodes and the adjacent arcs by a line consisting of j arcs and j–1 meagre nodes with indices n–j+1, n–j+2,...,n–1 as in Fig. 1, and put $t_{(1)}$ to the free end of this line.

Since the P-trees considered in [5] are related to the j-th part of (50) by the index j of the root $(1 \leqslant j \leqslant n)$, only P-trees belonging to Y_n are given above. To get the P-trees relative to $Y_j (1 \leqslant j \leqslant n-1)$, a descending line of n–j arcs and meagre nodes labelled as in fig. 2 is put to the root of each tree t_G. The resulting trees are denoted by t_{jG}, where the new root is the lowest node of t_{jG} with index j. Hence, all trees of TN which remain after assuming (40) are known.



$t_G = t_{nG}$ $\qquad$ t_{jG} $(j<n)$

Fig. 2. P-trees relative to the function Y_j $(1 \leqslant j \leqslant n)$.

Interpreting lemma 16 by Hairer [5] for the partitioned system (50) with (51), one can find the order conditions relative to each P-tree immediately by the following instructions as done in [7] for n=2 :

To each fat node of a P-tree t with root-index j attach a summation letter $\kappa,\lambda,\mu,...$. Then, the order condition relative to t takes the form

$$\gamma(t) \cdot \sum_{\kappa,\lambda,\mu,...} c_\kappa^{(n-j+1)} . \Phi = 1, \tag{52}$$

where Φ is a product containing the factors

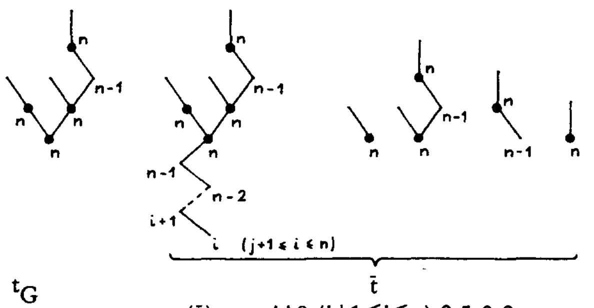
$\beta_{\kappa\lambda}^{(j)}$ whenever a lower fat node "κ" is connected with a higher fat node "λ" by j arcs without other fat nodes between them;

a_κ^q whenever the fat node "κ" is directly connected with q meagre end-nodes.

If $\rho(t)$ denotes the total number of all nodes (fat ones and meagre ones) of t, $\gamma(t)$ finally results as the product of all $\rho(\bar{t})$, where $\bar{t}$ represents all P-trees (inclusive t) which are got, if one root after the other and the adjacent arcs are left away.

Example 18

We consider the P-tree $t_{(j+1)G}$ relative to $Y^{(j)} = Y_{j+1}$ corresponding to G = (0|1,1)(1)((1|2)(1)) from



$\rho(\bar{t}) = n-i+8$ $(j+1 \leqslant i \leqslant n)$,2,5,3,2

Fig. 3. Subtrees occuring in $t_{(j+1)G}$ from example 18.

examples 5 and 17.

By the above instructions we get

$$\gamma(t_{(j+1)G}) = \prod_{i=j+1}^{n} (n-i+8).2.5.3.2 = \frac{1}{84}.(n-j+7)!. \tag{53}$$

Therefore the condition

$$1 = \frac{1}{84}.(n-j+7)! . \sum_{\kappa,\lambda,\mu,\nu} c_\kappa^{(n-j)} \beta_{\kappa\lambda}^{(1)} a_\lambda \beta_{\kappa\mu}^{(1)} a_\mu \beta_{\mu\nu}^{(2)} a_\nu \tag{54}$$

resulting from (52) is identical to (49).

Thus, there are two different ways to find the order conditions for Runge-Kutta-Nyström methods, applicable to systems of n-th order differential equations.

5. APPLICATION TO RUNGE-KUTTA-FEHLBERG METHODS

By a p-fold differentiation of the given system of differential equations (1) to get the extended initial values $Y_0^{(n)},...,Y_0^{(n+p)}$ $(p \geqslant 0)$, and by the transformation

$$Y(x) = \bar{Y}(x) + \sum_{j=1}^{n+p} \frac{1}{j!} (x-x_0)^j Y_0^{(j)}, \tag{55}$$

Fehlberg [9] obtained some Runge-Kutta formulas whose order was increased by p as against the order of classical Runge-Kutta-Nyström methods without multiplying the stages. The function evaluation $\bar{F}_0$ in (2) and (3) even may be omitted. This follows, since the initial values of the "transformed" system of differential equations

$$\bar{Y}^{(n)} = \bar{F}(x,\bar{Y},\bar{Y}',...,\bar{Y}^{(n-1)}) \tag{56}$$

satisfy the conditions

$$\bar{Y}_0 = Y_0, \bar{Y}_0' = \bar{Y}_0'' = ... = \bar{Y}_0^{(n+p)} = 0. \tag{57}$$

Thus the corresponding elementary differentials of orders $u \leqslant p$ and those which include such an elementary differential as any "factor", vanish at x_0. In the comparison of the Taylor series of both the exact solution and approximation, the conditions for the Runge-Kutta coefficients, generated by the above elementary differentials, no more must be satisfied.

TABLE 2

Conditions for Runge-Kutta-Nyström (p=0) and Runge-Kutta-Fehlberg methods up to order p+4 (for all conditions up to order p+7 see [12]).

No.	u	elementary differential	condition for the R-K coefficients relative to $Y^{(n-j)}$ $(1\leq j\leq n)$	
1	0	(0)	$\sum_\kappa c_\kappa^{(j)}$	$=\frac{1}{j!}$
2	p+1	(p+1)	$\sum_\kappa c_\kappa^{(j)}\,a_\kappa^{p+1}$	$=\frac{(p+1)!}{(p+1+j)!}$
3	p+2	(p+2)	$\sum_\kappa c_\kappa^{(j)}\,a_\kappa^{p+2}$	$=\frac{(p+2)!}{(p+2+j)!}$
4		(0|1)(p+1)	$\sum_\kappa c_\kappa^{(j)}\sum_\lambda \beta_{\kappa\lambda}^{(1)}\,a_\lambda^{p+1}$	$=\frac{(p+1)!}{(p+2+j)!}$
5	p+3	(p+3)	$\sum_\kappa c_\kappa^{(j)}\,a_\kappa^{p+3}$	$=\frac{(p+3)!}{(p+3+j)!}$
6		(0|1)(p+2)	$\sum_\kappa c_\kappa^{(j)}\sum_\lambda \beta_{\kappa\lambda}^{(1)}\,a_\lambda^{p+2}$	$=\frac{(p+2)!}{(p+3+j)!}$
7		(1|1)(p+1)	$\sum_\kappa c_\kappa^{(j)}\,a_\kappa\sum_\lambda \beta_{\kappa\lambda}^{(1)}\,a_\lambda^{p+1}$	$=\frac{(p+3)(p+1)!}{(p+3+j)!}$
8		$(0\|1)^2$(p+1)	$\sum_\kappa c_\kappa^{(j)}\sum_\lambda \beta_{\kappa\lambda}^{(1)}\sum_\mu \beta_{\lambda\mu}^{(1)}\,a_\mu^{p+1}$	$=\frac{(p+1)!}{(p+3+j)!}$
9		(0|2)(p+1)	$\sum_\kappa c_\kappa^{(j)}\sum_\lambda \beta_{\kappa\lambda}^{(2)}\,a_\lambda^{p+1}$	$=\frac{(p+1)!}{(p+3+j)!}$
10	p+4	(p+4)	$\sum_\kappa c_\kappa^{(j)}\,a_\kappa^{p+4}$	$=\frac{(p+4)!}{(p+4+j)!}$
11		(0|1)(p+3)	$\sum_\kappa c_\kappa^{(j)}\sum_\lambda \beta_{\kappa\lambda}^{(1)}\,a_\lambda^{p+3}$	$=\frac{(p+3)!}{(p+4+j)!}$
12		(1|1)(p+2)	$\sum_\kappa c_\kappa^{(j)}\,a_\kappa\sum_\lambda \beta_{\kappa\lambda}^{(1)}\,a_\lambda^{p+2}$	$=\frac{(p+4)(p+2)!}{(p+4+j)!}$
13		(2|1)(p+1)	$\sum_\kappa c_\kappa^{(j)}\,a_\kappa^2\sum_\lambda \beta_{\kappa\lambda}^{(1)}\,a_\lambda^{p+1}$	$=\frac{(p+4)(p+3)(p+1)!}{(p+4+j)!}$
14		$(0\|1)^2$(p+2)	$\sum_\kappa c_\kappa^{(j)}\sum_\lambda \beta_{\kappa\lambda}^{(1)}\sum_\mu \beta_{\lambda\mu}^{(1)}\,a_\mu^{p+2}$	$=\frac{(p+2)!}{(p+4+j)!}$
15		(0|1)(1|1)(p+1)	$\sum_\kappa c_\kappa^{(j)}\sum_\lambda \beta_{\kappa\lambda}^{(1)}\,a_\lambda\sum_\mu \beta_{\lambda\mu}^{(1)}\,a_\mu^{p+1}$	$=\frac{(p+3)(p+1)!}{(p+4+j)!}$
16		(1|1)(0|1)(p+1)	$\sum_\kappa c_\kappa^{(j)}\,a_\kappa\sum_\lambda \beta_{\kappa\lambda}^{(1)}\sum_\mu \beta_{\lambda\mu}^{(1)}\,a_\mu^{p+1}$	$=\frac{(p+4)(p+1)!}{(p+4+j)!}$
17		$(0\|1)^3$(p+1)	$\sum_\kappa c_\kappa^{(j)}\sum_\lambda \beta_{\kappa\lambda}^{(1)}\sum_\mu \beta_{\lambda\mu}^{(1)}\sum_\nu \beta_{\mu\nu}^{(1)}\,a_\nu^{p+1}$	$=\frac{(p+1)!}{(p+4+j)!}$
18		$(0\|1,1)(1)^2$	$\sum_\kappa c_\kappa^{(j)}\,(\sum_\lambda \beta_{\kappa\lambda}^{(1)}\,a_\lambda)^2$	$=\frac{6}{(4+j)!}$
19		(0|2)(p+2)	$\sum_\kappa c_\kappa^{(j)}\sum_\lambda \beta_{\kappa\lambda}^{(2)}\,a_\lambda^{p+2}$	$=\frac{(p+2)!}{(p+4+j)!}$
20		(1|2)(p+1)	$\sum_\kappa c_\kappa^{(j)}\,a_\kappa\sum_\lambda \beta_{\kappa\lambda}^{(2)}\,a_\lambda^{p+1}$	$=\frac{(p+4)(p+1)!}{(p+4+j)!}$
21		(0|1)(0|2)(p+1)	$\sum_\kappa c_\kappa^{(j)}\sum_\lambda \beta_{\kappa\lambda}^{(1)}\sum_\mu \beta_{\lambda\mu}^{(2)}\,a_\mu^{p+1}$	$=\frac{(p+1)!}{(p+4+j)!}$

No.	u	elementary differential	condition for the R-K coefficients relative to $Y^{(n-j)}$ $(1\leq j\leq n)$
22	p + 4	(0|2)(0|1)(p+1)	$\sum_{\kappa} c_{\kappa}^{(j)} \sum_{\lambda} \beta_{\kappa\lambda}^{(2)} \sum_{\mu} \beta_{\lambda\mu}^{(1)} a_{\mu}^{p+1} = \frac{(p+1)!}{(p+4+j)!}$
23		(0|3)(p+1)	$\sum_{\kappa} c_{\kappa}^{(j)} \sum_{\lambda} \beta_{\kappa\lambda}^{(3)} a_{\lambda}^{p+1} = \frac{(p+1)!}{(p+4+j)!}$
The lower and upper bounds of the variables, κ,λ,μ and ν are omitted. The first condition is only to consider in classical Runge-Kutta-Nyström methods. Condition No. 18 only must be satisfied for p=0.			

TABLE 3

Coefficients for a three-stage formula, applicable to the system $Y^{(n)} = F(x,Y,Y',...,Y^{(n-1)})$.

$$a_1 = a_2 = \frac{p+2}{p+4},\quad a_3 = 1;$$

$$\beta_{21}^{(1)} = \frac{3(p+4)^{p+1}}{2(p+2)^{p+2}(p+3)},\quad \beta_{31}^{(1)} = \frac{(p+4)^{p+1}}{(p+2)^{p+2}} - \frac{4(p+3)}{3(p+4)},$$

$$\beta_{32}^{(1)} = \frac{4(p+3)}{3(p+4)},\quad \beta_{21}^{(2)} = \frac{3(p+4)^{p}}{(p+2)^{p+2}(p+3)} - \frac{3}{4(p+3)},\quad \beta_{32}^{(2)} = \frac{1}{2}$$

$$c_1^{(j)} = \frac{j}{(p+2+j)!}\left[\frac{(p+4)^{p+2}(p+1)!}{2(p+2)^{p+1}} - \frac{(p+3)!}{3}\right],$$

$$c_2^{(j)} = \frac{j(p+3)!}{3(p+2+j)!},\quad c_3^{(j)} = \frac{(2-j)(p+2)!}{2(p+2+j)!}\quad (1\leq j\leq n).$$

$$[c_0^{(j)} = \frac{j^2}{(2+j)!},\quad \beta_{10}^{(j)} = \frac{1}{2^j.j!}\quad (1\leq j\leq n);\quad \beta_{20}^{(2)} = \frac{1}{8}.]$$

TABLE 4

Coefficients for a two-stage formula, applicable to the special system $Y^{(n)} = F(x,Y,Y',...Y^{(n-2)})$ which does not depend on $Y^{(n-1)}$.

$$a_1 = \frac{p+2}{p+4},\quad a_2 = 1;\quad \beta_{21}^{(2)} = \frac{2(p+4)^{p}}{(p+2)^{p+2}}$$

$$c_1^{(j)} = \frac{j(p+4)^{p+2}(p+1)!}{2(p+2)^{p+1}(p+2+j)!},\quad c_2^{(j)} = \frac{(2-j)(p+2)!}{2(p+2+j)!}\quad (1\leq j\leq n).$$

$$[c_0^{(j)} = \frac{j^2}{(2+j)!}\quad (1\leq j\leq n),\quad \beta_{10}^{(j)} = \frac{1}{2^j.j!}\quad (2\leq j\leq n).]$$

In particular, this is true for equation (40), so that this assumption no more must be made to apply definition 13.
The order of those elementary differentials which furthermore have to be considered, is at least u=p+1. In the case where p is chosen very high or even remains variable, the determination of the Runge-Kutta conditions by the classical way of successive differentiation is very complicated. However, the formulas of theorems 12 and 16 are universally applicable. This is also valid for equation (52), if the corresponding P-trees are determined.
In table 2 we present all those elementary differentials of orders p+1 until p+4 which occur in the Taylor expansions of $\bar{Y}^{(j)}(x_0+h)$ and $\bar{Y}_h^{(j)}(0\leq j\leq n-1)$ of the transformed system (56).

To get a Runge-Kutta-Fehlberg method of order p+q for each derivative $Y^{(n-j)}$ $(1 \leq j \leq n)$, only those conditions of table 2 have to be satisfied for computing $\overline{Y}_h^{(n-j)}$, which are created by the elementary differentials of orders $p+1$ until $p+q-j$. In the case that the Runge-Kutta scheme is explicit, it may be necessary to choose the number of function evaluations $\overline{F}_\kappa$ (respectively F_κ in Nyström methods) in (2) sufficiently high to guarantee the existence of all elementary differentials up to the desired order in the Taylor series of the approximation. Considering classical Runge-Kutta-Nyström algorithms the special case $p=0$ is valid, and additionally the condition generated by $G=(0)$ has to be satisfied. Then the conditions of table 2 are identical to those of Bettis [6].

Example 19

Finally we present two explicit Runge-Kutta-Fehlberg formulas of order p+4 ($p \geq 0$ may be arbitrary). The first one is a threestage algorithm whose coefficients are listed in table 3. Those coefficients which are listed in brackets, have only to be considered in Runge-Kutta-Nyström methods. In this case we obtain the algorithm by Zurmühl [8]. The two-stage method, characterized by the coefficients of table 4, is applicable to special systems of the form

$$Y^{(n)} = F(x,Y,Y',\ldots,Y^{(n-2)}) \tag{58}$$

which do not depend on $Y^{(n-1)}$. For $p=0$ the coefficients of table 4 are the same as in Albrecht [11]. All coefficients not mentioned in tables 3 and 4 are set to zero.

In a forthcoming paper we will consider some extended Runge-Kutta-Fehlberg methods (see [13,14]). A further extension of these methods enables us to construct a new transformation similar to (55). In contrast to the given system (1) the transformed system (56) of the new method no more depends on $\overline{Y}^{(n-1)}$. Hence, some simplified Runge-Kutta schemes may be used. Some explicit formulas are presented and applied to some numerical examples.

REFERENCES

1. BUTCHER J. C. : "Coefficients for the study of Runge-Kutta integration processes", J. Austral. Math. Soc., Vol. 3, 1963, pp. 185-201.

2. KASTLUNGER K., WANNER G. : "On Turan type implicit Runge-Kutta methods", Computing, Vol. 9, 1972, pp. 317-325.

3. HAIRER E., WANNER G. : "Multistep-multistage-multiderivative methods for ordinary differential equations", Computing, Vol. 11, 1973, pp. 287-303.

4. HAIRER E., WANNER G. : "On the Butcher group and general multi-value methods", Computing, Vol. 13, 1974, pp. 1-15.

5. HAIRER E. : "Order conditions for numerical methods for partitioned ordinary differential equations", Numer. Math., Vol. 36, 1981, pp. 431-445.

6. BETTIS D. G. : "Equations of condition for high order Runge-Kutta-Nyström formulae", Lecture Notes in Mathematics, Vol. 362, 1972, pp. 76-91.

7. HAIRER E., WANNER G. : "A theory for Nyström methods", Numer. Math., Vol. 25, 1976, pp. 383-400.

8. ZURMÜHL R. : "Runge-Kutta-Verfahren zur numerischen Integration von Differentialgleichungen n-ter Ordnung", Z. angew. Math. Mech., Vol. 28, 1948, pp. 173-182.

9. FEHLBERG E. : "New high order Runge-Kutta formulas with step size control for systems of first- and second order differential equations", Z. angew. Math. Mech., Vol. 44, 1964, pp. T17-T29.

10. COLLATZ L. : *The numerical treatment of differential equations,* Springer, Berlin-Heidelberg-New York, 1966.

11. ALBRECHT J. : "Beiträge zum Runge-Kutta-Verfahren", Z. angew. Math. Mech., Vol. 35, 1955, pp. 100-110.

12. HEBSAKER H.-M. : "Neue Runge-Kutta-Fehlberg-Verfahren für Differentialgleichungs-Systeme n-ter Ordnung", Thesis, Siegen, 1980, 266 pp.

13. FEHLBERG E. : "Neue genauere Runge-Kutta-Formeln für Differentialgleichungen n-ter Ordnung", Z. angew. Math. Mech., Vol. 40, 1960, pp. 449-455.

14. COTIU A. : "Procedee de tip Runge-Kutta, de ordin inalt de exactitate, de integrare numerica a ecuatiilor diferentiale de ordinul n", Bul. Stiint. Inst. Politehn. Cluj, Vol. 13, 1973, pp. 19-24.