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ORDER CONDITIONS FOR A CLASS OF RUNGE-KUTTA-ROSENBROCK METHODS

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Order conditions for a class of Runge-Kutta-Rosenbrock methods

by

J.G. Blom

ABSTRACT

This report deals with the derivation of the order conditions for a class of Runge-Kutta-Rosenbrock methods for stiff differential equations that is described in [5]. Recurrence relations for the order conditions are obtained by a technique similar to that used by WOLFBRANDT [6]. The order conditions are generated by an ALGOL 68 program and are listed up to order 6.

KEY WORDS & PHRASES: *Numerical analysis, stiff systems of ordinary differential equations, Runge-Kutta-Rosenbrock methods*

1. INTRODUCTION

This report deals with the derivation of order conditions for a Runge-Kutta-Rosenbrock (RKR) method which has been developed for the numerical solution of the initial value problem for stiff systems of ordinary differential equations

$$(1.1)\qquad \frac{d\vec{y}}{dx} = f(\vec{y}) \qquad x \geq x_0,\ \vec{y}(x_0) = \vec{y}_0.$$

The RKR method has been discussed in [5] and is given by (cf. formula 2.3 in [5]):

$$(1.2)\qquad \begin{cases} [I - \gamma h \frac{\partial \vec{f}}{\partial \vec{y}}(\vec{y}_{n+\eta})]\vec{k}_i = \vec{f}\left(\vec{y}_n + h \sum\limits_{j=1}^{i-1} \alpha_{ij}\vec{k}_j\right) + \\ \qquad\qquad + h \frac{\partial \vec{f}}{\partial \vec{y}}(\vec{y}_{n+\eta}) \sum\limits_{j=1}^{i-1} \gamma_{ij}\, \vec{k}_j, \qquad i = 1,\dots,s \\ \vec{y}_{n+1} = \vec{y}_n + h \sum\limits_{i=1}^{s} \mu_i \vec{k}_i, \end{cases}$$

where α_{ij}, γ_{ij}, μ_i and γ are real parameters and η a non-positive integer.

In analogy to WOLFBRANDT [6] we expand the solution $\vec{y}(x_n+h)$ in a Taylor series and compare term by term with the expansion of the approximate solution $\vec{y}_{n+1}$. In that way we obtain recurrence relations for the order conditions with parameters α_{ij}, γ_{ij}, μ_i, γ and η. For these expansions and for the generation of the order conditions from the recurrence relations we make use of the theory of the elementary differentials formulated by BUTCHER ([1] and [2]).

In Chapter 2 we will give some preliminaries on this theory that we need for the evaluation of the recurrence relations and derive these relations themselves. For the generation of the order conditions from the recurrence relations we did write a computer program that is based on the correspondence between elementary differentials and rooted trees. An outline of this program will be discussed in Chapter 3. There we also list the order conditions up to order 6.

2. RECURRENCE RELATIONS FOR THE ORDER CONDITIONS

2.1. Elementary differentials

The theory of elementary differentials has been formulated by BUTCHER [1]. This section will contain some notations, a definition and a theorem that are needed to understand the remainder of the chapter. For further details and proofs we refer to BUTCHER [1].

DEFINITION 2.1.1. For a mapping $\vec{f}: \mathbb{R}^N \to \mathbb{R}^N$ the elementary differentials $\vec{F}: \mathbb{R}^N \to \mathbb{R}^N$ of given order and degree are recursively defined as:

$\vec{f}$ is the only elementary differential of order 1;
the degree is not defined.

$\vec{F}$ is an elementary differential of order r and degree s

if

$$\vec{F} = \sum_{j_1=1}^{N} \sum_{j_2=1}^{N} \cdots \sum_{j_s=1}^{N} \frac{\partial^s \vec{f}}{\partial y_{j_1} \partial y_{j_2} \cdots \partial y_{j_s}} F_{1j_1} F_{2j_2} \cdots F_{sj_s},$$

where F_{ij} is the j-th component of an elementary differential $\vec{F}_i$ of order r_i $(i = 1,2,\ldots,s)$ such that

$$r = 1 + \sum_{i=1}^{s} r_i.$$

This elementary differential will be written as $\vec{F} = \{\vec{F}_1\vec{F}_2\ldots\vec{F}_s\}$.

Note that in general $\vec{F}_1,\vec{F}_2,\ldots,\vec{F}_s$ need not be distinct.

Each elementary differential of $\vec{f}$ is denoted by a string of letters and bracket symbols. As abbreviations will be used:

$$\underbrace{\vec{F}\ldots\vec{F}}_{k} = \vec{F}^k, \quad \underbrace{\{\{\ldots\{}_{k} = \{_k \quad \text{and} \quad \underbrace{\}\}\ldots\}}_{k} = \}_k .$$

THEOREM 2.1.1. *Let* D *be a differential operator defined by*

$$D = \sum_{j=1}^{N} f_j \frac{\partial}{\partial y_j},$$

where $\vec{f}$ *is defined by* (1.1). *Then* $D^{r-1}\vec{f}$ *is a linear combination with positive integer coefficients of the elementary differentials of order* r.

$$D^{r-1}\vec{f} = \sum_{\text{ord } \vec{F} = r} \kappa(\vec{F})\vec{F}.$$

If $\vec{F} = \{\vec{F}_1^{\nu_1}\vec{F}_2^{\nu_2} \ldots \vec{F}_\sigma^{\nu_\sigma}\}$ *with* $\vec{F}_1, \vec{F}_2, \ldots, \vec{F}_\sigma$ *all distinct, then the coefficient* κ *of* $\vec{F}$ *satisfies:*

$$\kappa(\vec{F}) = (r-1)! \prod_{i=1}^{\sigma} \frac{1}{\nu_i!}\left(\frac{\kappa(\vec{F}_i)}{r_i!}\right)^{\nu_i}, \tag{2.1.1}$$

where r_i *is the order of* $\vec{F}_i$ *and* $\kappa(\vec{f}) = 1$.

2.2. Taylor expansion of $\vec{y}$

If we expand the solution $\vec{y}(x_n+h)$ of (1.1) in a Taylor series about the point x_n assuming that $\vec{y}(x_n) = \vec{y}_n$, we find

$$\vec{y}(x_n+h) = \vec{y}_n + \sum_{r=1}^{\infty} \frac{h^r}{r!} [D^{r-1}\vec{f}]_n,$$

where $[\vec{A}]_n$ denotes $\vec{A}(\vec{y}_n)$. By application of Theorem 2.1.1 this can be written as

$$\vec{y}(x_n+h) = \vec{y}_n + \sum_{r=1}^{\infty} \frac{h^r}{r!} \sum_{\text{ord } \vec{F} = r} \kappa(\vec{F})[\vec{F}]_n, \tag{2.2.1}$$

where the coefficient κ is given by (2.1.1).

2.3. Expansion of the approximate solution

For the sake of simplicity we first restrict our attention to the scalar equation

$$\frac{dy}{dx} = f(y), \quad x > x_n, \; y(x_n) = y_n. \tag{2.3.1}$$

The RKR method then reads

$$(2.3.2)\quad \begin{cases} \text{(a)}\; k_i = [1-\gamma h \frac{df}{dy}(y_{n+\eta})]^{-1}\Big\{f\Big(y_n + h \sum_{j=1}^{i-1} \alpha_{ij}k_j\Big) + \\ \qquad + h\frac{df}{dy}(y_{n+\eta})\sum_{j=1}^{i-1}\gamma_{ij}k_j\Big\}, \quad i = 1,\dots,s \\ \text{(b)}\; y_{n+1} = y_n + h\sum_{i=1}^{s}\mu_i k_i. \end{cases}$$

If h is small enough, k_i can be expanded in a power series:

$$(2.3.3)\qquad k_i = \sum_{r=0}^{\infty}\frac{h^r}{r!}K_{i,r}.$$

<u>LEMMA 2.3.1</u>. *Let* $f = f(y)$ *be analytic and let* $y_{n+\eta}$ *have an expansion of the form*

$$y_{n+\eta} = y_n + \sum_{r=1}^{\infty} h^r z_r,$$

where, since η *is a non-positive integer,*

$$z_r = \frac{\eta^r}{r!}[D^{r-1}f]_n.$$

Then the recurrence relation for $K_{i,r}$ *is:*

$$K_{i,0} = [f]_n,$$

$$(2.3.4)\qquad K_{i,r} = \sum_{k=1}^{r}\frac{r!}{k!}\sum_{r_1+\dots+r_k=r}\Big(\prod_{m=1}^{k}\sum_{j=1}^{i-1}\alpha_{ij}\frac{K_{j,r_m-1}}{(r_m-1)!}\Big)\Big[\frac{d^kf}{dy^k}\Big]_n +$$

$$+ r\Big(\sum_{j=1}^{i-1}\gamma_{ij}K_{j,r-1} + \gamma K_{i,r-1}\Big)\Big[\frac{df}{dy}\Big]_n +$$

$$+ \sum_{q=1}^{r-1}\sum_{k=1}^{q}\frac{r!}{k!}\sum_{r_1+\dots+r_k=q}\Big(\prod_{m=1}^{k} z_{r_m}\Big)\cdot$$

$$\cdot\Big(\sum_{j=1}^{i-1}\gamma_{ij}\frac{K_{j,r-q-1}}{(r-q-1)!} + \gamma\frac{K_{i,r-q-1}}{(r-q-1)!}\Big)\Big[\frac{d^{k+1}f}{dy^{k+1}}\Big]_n.$$

PROOF. The identity $K_{i,0} = [f]_n$ is trivially satisfied. In order to get the recurrence relation for $K_{i,r}$ with $r > 0$ we replace k_j by the corresponding power series (2.3.3) and expand step by step all terms of the equation (2.3.2.a)

$$h \sum_{j=1}^{i-1} \gamma_{ij} k_j = h \sum_{j=1}^{i-1} \gamma_{ij} \sum_{r=0}^{\infty} \frac{h^r}{r!} K_{j,r} =$$

$$= \sum_{r=1}^{\infty} h^r \sum_{j=1}^{i-1} \gamma_{ij} \frac{K_{j,r-1}}{(r-1)!} \overset{\text{not.}}{=\!=} \sum_{r=1}^{\infty} h^r c_{i,r},$$

$$y_n + h \sum_{j=1}^{i-1} \alpha_{ij} k_j = y_n + \sum_{r=1}^{\infty} h^r \sum_{j=1}^{i-1} \alpha_{ij} \frac{K_{j,r-1}}{(r-1)!} \overset{\text{not.}}{=\!=} y_n + \sum_{r=1}^{\infty} h^r a_{i,r}.$$

By using Taylor's theorem and the multinomial theorem we obtain the power series for

$$f\left(y_n + h \sum_{j=1}^{i-1} \alpha_{ij} k_j\right) = [f]_n + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{r=1}^{\infty} h^r a_{i,r}\right)^k \left[\frac{d^k f}{dy^k}\right]_n =$$

$$= [f]_n + \sum_{r=1}^{\infty} h^r \sum_{k=1}^{r} \frac{1}{k!} \sum_{r_1+\ldots+r_k=r}$$

$$\left(\prod_{m=1}^{k} a_{i,r_m}\right)\left[\frac{d^k f}{dy^k}\right]_n \overset{\text{not.}}{=\!=} [f]_n +$$

$$+ \sum_{r=1}^{\infty} h^r \sum_{k=1}^{r} \frac{1}{k!} S(r,k,a_i) \left[\frac{d^k f}{dy^k}\right]_n$$

and for

$$\frac{df}{dy}(y_{n+\eta}) = [\frac{df}{dy}]_n + \sum_{k=1}^{\infty} \frac{1}{k!} \left\{\sum_{r=1}^{\infty} h^r z_r\right\}^k \left[\frac{d^{k+1} f}{dy^{k+1}}\right]_n =$$

$$= [\frac{df}{dy}]_n + \sum_{r=1}^{\infty} h^r \sum_{k=1}^{r} \frac{1}{k!} \sum_{r_1+\ldots+r_k=r} \left(\prod_{m=1}^{k} z_{r_m}\right)\left[\frac{d^{k+1} f}{dy^{k+1}}\right]_n$$

$$\overset{\text{not.}}{=\!=} [\frac{df}{dy}]_n + \sum_{r=1}^{\infty} h^r \sum_{k=1}^{r} \frac{1}{k!} S(r,k,z) \left[\frac{d^{k+1} f}{dy^{k+1}}\right]_n .$$

With these relations we can expand the right-hand side of equation (2.3.2.a). Let

$$A = 1 - \gamma h \frac{df}{dy}(y_{n+\eta}) =$$

$$= 1 - \gamma h \frac{df}{dy}(y_n) - \gamma \sum_{r=2}^{\infty} h^r \sum_{k=1}^{r-1} \frac{1}{k!} S(r-1,k,z)\left[\frac{d^{k+1}f}{dy^{k+1}}\right]_n$$

and

$$B = f\left(y_n + h\sum_{j=1}^{i-1} \alpha_{ij}k_j\right) + h\frac{df}{dy}(y_{n+\eta})\sum_{j=1}^{i-1} \gamma_{ij}k_j =$$

$$= [f]_n + \sum_{r=1}^{\infty} h^r \left\{\sum_{k=1}^{r} \frac{1}{k!} S(r,k,a_i)\left[\frac{d^k f}{dy^k}\right]_n + [\tfrac{df}{dy}]_n\, c_{i,r} + \right.$$

$$\left. + \sum_{q=1}^{r-1}\left(\sum_{k=1}^{q} \frac{1}{k!} S(q,k,z)\left[\frac{d^{k+1}f}{dy^{k+1}}\right]_n\right)c_{i,r-q}\right\}.$$

Then using the relation for the quotient of two power series

$$\sum_{r=0}^{\infty} \beta_r x^r \Big/ \sum_{r=0}^{\infty} \alpha_r x^r = \sum_{r=0}^{\infty} \gamma_r x^r,$$

where

$$\gamma_r = \beta_r - \sum_{q=0}^{r-1} \gamma_q \alpha_{r-q}, \qquad \text{if } \alpha_0 = 1,$$

we get for the right-hand side of (2.3.2.a):

$$A^{-1}B = \sum_{r=0}^{\infty} h^r b_r$$

with

$$b_0 = [f]_n,$$

$$b_r = \sum_{k=1}^{r} \frac{1}{k!} S(r,k,a_i)\left[\frac{d^k f}{dy^k}\right]_n + [\tfrac{df}{dy}]_n\, c_{i,r} +$$

$$+ \sum_{q=1}^{r-1}\left(\sum_{k=1}^{q} \frac{1}{k!} S(q,k,z)\left[\frac{d^{k+1}f}{dy^{k+1}}\right]_n\right) c_{i,r-q} +$$

$$+\sum_{q=0}^{r-2} b_q\gamma \sum_{k=1}^{r-q-1} \frac{1}{k!} S(r-q-1,k,z)\left[\frac{d^{k+1}f}{dy^{k+1}}\right]_n + b_{r-1}\gamma\left[\frac{df}{dy}\right]_n.$$

From equations (2.3.3) and (2.3.2.a) it follows that

$$\sum_{r=0}^{\infty} h^r \frac{K_{i,r}}{r!} = \sum_{r=0}^{\infty} h^r b_r.$$

So the recurrence relation for $K_{i,r}$ for $r > 0$ becomes:

$$K_{i,r} = r!\left\{\sum_{k=1}^{r} \frac{1}{k!} \sum_{r_1+\ldots+r_k=r} \left(\prod_{m=1}^{k} \sum_{j=1}^{i-1} \alpha_{ij} \frac{K_{j,r_m-1}}{(r_m-1)!}\left[\frac{d^k f}{dy^k}\right]_n\right. + \right.$$

$$+ \sum_{j=1}^{i-1} \gamma_{ij} \frac{K_{j,r-1}}{(r-1)!} \left[\frac{df}{dy}\right]_n +$$

$$+ \sum_{q=1}^{r-1}\left(\sum_{k=1}^{q} \frac{1}{k!} \sum_{r_1+\ldots+r_k=q} \left(\prod_{m=1}^{k} z_{r_m}\right)\right)\left(\sum_{j=1}^{i-1} \gamma_{ij} \frac{K_{j,r-q-1}}{(r-q-1)!}\right)\left[\frac{d^{k+1}f}{dy^{k+1}}\right]_n +$$

$$\left. + \gamma \sum_{q=0}^{r-2} \frac{K_{i,q}}{q!} \sum_{k=1}^{r-q-1} \frac{1}{k!} \sum_{r_1+\ldots+r_k=r-q-1} \left(\prod_{m=1}^{k} z_{r_m}\right)\left[\frac{d^{k+1}f}{dy^{k+1}}\right]_n + \gamma \frac{K_{i,r-1}}{(r-1)!}\left[\frac{df}{dy}\right]_n\right\},$$

which, after a little manipulation, is equal to (2.3.4). □

We next proof that $K_{i,r-1}$ can be expressed as a linear combination of the elementary differentials of order r.

<u>LEMMA 2.3.2.</u> *Under the conditions of Lemma* 2.3.1, $K_{i,r-1}$ *can be written as*

(2.3.5) $$K_{i,r-1} = \sum_{\operatorname{ord} F = r} \psi_i(F)[F]_n,$$

where $\psi_i(F)$ *is a polynomial in* α_{ij}, γ_{ij}, γ *and* η *that satisfies the recurrence relation:*

(2.3.6)

if order F *is* 1: $\psi_i(f) = 1$,

if order F *is* r *and* $F = \{F_1^{\nu_1}\ldots F_\sigma^{\nu_\sigma}\}$ *with* F_i *all distinct for* $i = 1,\ldots,\sigma$*:* $\psi_i(F) =$

$$= (r-1)! \prod_{m=1}^{\sigma} \frac{1}{\nu_m!}\left(\frac{1}{r_m!}\right)^{\nu_m} \left\{ \prod_{m=1}^{\sigma} \left(\sum_{j=1}^{i-1} \alpha_{ij} r_m \psi_j(F_m) \right)^{\nu_m} + \right.$$

$$\left. + \prod_{m=1}^{\sigma} (\eta^{r_m} \kappa(F_m))^{\nu_m} \sum_{q=1}^{\sigma} \frac{\nu_q r_q}{\eta^{r_q} \kappa(F_q)} \left(\sum_{j=1}^{i-1} \gamma_{ij} \psi_j(F_q) + \gamma \psi_i(F_q) \right) \right\}.$$

PROOF. We will proof this lemma by mathematical induction on r. If $r = 1$ then $K_{i,0} = [f]_n$; when we take $\psi_i(f) = 1$ then relation (2.3.5) is satisfied. Assume that (2.3.5) holds for $r = 1,2,\ldots,\bar{r}-1$, $\bar{r} \geq 2$. To prove the lemma for $r = \bar{r}$ we firstly recall that

$$z_r = \frac{\eta^r}{r!}[D^{r-1}f]_n = \frac{\eta^r}{r!} \sum_{\mathrm{ord}\,F = r} \kappa(F)[F]_n$$

with κ given by (2.1.1). When we substitute this in (2.3.4) and use the induction hypothesis, we find for $K_{i,\bar{r}-1}$

$$\text{(2.3.7)} \qquad K_{i,\bar{r}-1} = \sum_{k=1}^{\bar{r}-1} \sum_{r_1+\ldots+r_k=\bar{r}-1} \sum_{\mathrm{ord}\,F_1 = r_1} \cdots \sum_{\mathrm{ord}\,F_k = r_k}$$

$$\frac{(\bar{r}-1)!}{k!} \left(\prod_{m=1}^{k} \sum_{j=1}^{i-1} \alpha_{ij} \frac{\psi_j(F_m)}{(r_m-1)!} \right) \left[F_1 \ldots F_k \frac{d^k f}{dy^k} \right]_n +$$

$$+ (\bar{r}-1) \sum_{\mathrm{ord}\,F_1 = \bar{r}-1} \left(\sum_{j=1}^{i-1} \gamma_{ij} \psi_j(F_1) + \gamma \psi_i(F_1) \right) \left[F_1 \frac{df}{dy} \right]_n +$$

$$+ \sum_{q=1}^{\bar{r}-2} \sum_{k=1}^{q} \sum_{r_1+\ldots+r_k=q} \sum_{\mathrm{ord}\,F_0 = \bar{r}-q-1} \sum_{\mathrm{ord}\,F_1 = r_1} \cdots \sum_{\mathrm{ord}\,F_k = r_k} \frac{(\bar{r}-1)!}{k!} \cdot$$

$$\cdot \left(\prod_{m=1}^{k} \frac{\eta^{r_m}}{r_m!} \kappa(F_m) \right) \left(\sum_{j=1}^{i-1} \gamma_{ij} \frac{\psi_j(F_0)}{(\bar{r}-q-2)!} + \gamma \frac{\psi_i(F_0)}{(\bar{r}-q-2)!} \right) \left[F_0 F_1 \ldots F_k \frac{d^{k+1} f}{dy^{k+1}} \right]_n .$$

After examination we find that the right-hand side of (2.3.7) is a sum of the $\bar{r}$-th order elementary differentials of f. To prove that $\psi_i(F)$ has the suggested form for all F of order $\bar{r}$, we distinguish three different types of elementary differentials of order $\bar{r}$.

a) $F = \{F_1\}$ and order $F_1 = \bar{r}-1$.

For these elementary differentials the right-hand side of (2.3.7) gives:

$$\sum_{\text{ord } F_1 = \bar{r}-1} (\bar{r}-1)!\left(\sum_{j=1}^{i-1} \alpha_{ij} \frac{\psi_j(F_1)}{(\bar{r}-2)!}\right)\left[F_1 \frac{df}{dy}\right]_n +$$

$$+ (\bar{r}-1) \sum_{\text{ord } F_1 = \bar{r}-1} \left(\sum_{j=1}^{i-1} \gamma_{ij}\psi_j(F_1) + \gamma\psi_i(F_1)\right)\left[F_1 \frac{df}{dy}\right]_n,$$

so

$$\psi_i(F) = (\bar{r}-1)\left\{\sum_{j=1}^{i-1}(\alpha_{ij}+\gamma_{ij})\psi_j(F_1) + \gamma\psi_i(F_1)\right\}.$$

b) $F = \{F_1^{\nu_1}\}$, $\nu_1 r_1 = \bar{r}-1$ with $\nu_1 > 1$ and r_1 the order of F_1.
For this type of elementary differentials the right-hand side of (2.3.7) is:

$$\left\{\sum_{\text{ord } F_1=r_1} \frac{(\bar{r}-1)!}{\nu_1!}\left(\sum_{j=1}^{i-1} \alpha_{ij} \frac{\psi_j(F_1)}{(r_1-1)!}\right)^{\nu_1} + \right.$$

$$\left.\sum_{\text{ord } F_1=r_1} \frac{(\bar{r}-1)!}{(\nu_1-1)!}\left(\frac{\eta^{r_1}}{r_1!}\kappa(F_1)\right)^{\nu_1-1}\left(\sum_{j=1}^{i-1} \gamma_{ij}\frac{\psi_j(F_1)}{(r_1-1)!} + \gamma\frac{\psi_i(F_1)}{(r_1-1)!}\right)\right\}\left[F_1^{\nu_1} \frac{d^{\nu_1}f}{dy^{\nu_1}}\right]_n$$

and

$$\psi_i(F) = \frac{(\bar{r}-1)!}{\nu_1!(r_1!)^{\nu_1}}\left\{\left(\sum_{j=1}^{i-1} \alpha_{ij} r_1 \psi_j(F_1)\right)^{\nu_1} + \right.$$

$$\left. + \nu_1 r_1 (\eta^{r_1}\kappa(F_1))^{\nu_1-1}\left(\sum_{j=1}^{i-1} \gamma_{ij}\psi_j(F_1) + \gamma\psi_i(F_1)\right)\right\}.$$

c) $F = \{F_1^{\nu_1} F_2^{\nu_2} \ldots F_\sigma^{\nu_\sigma}\}$, $\sum_{i=1}^{\sigma} \nu_i r_i = \bar{r}-1$ with $\sigma > 1$ and r_i the order of F_i. Then the right-hand side of (2.3.7) becomes:

$$\frac{(\bar{r}-1)!}{\prod_{m=1}^{\sigma} \nu_m!}\left\{\sum_{\text{ord } F_1=r_1} \cdots \sum_{\text{ord } F_\sigma=r_\sigma} \prod_{m=1}^{\sigma} \left(\sum_{j=1}^{i-1} \alpha_{ij} \frac{\psi_j(F_m)}{(r_m-1)!}\right)^{\nu_m} + \right.$$

$$\sum_{q=1}^{\sigma} \sum_{\text{ord } F_1=r_1} \cdots \sum_{\text{ord } F_\sigma=r_\sigma} \prod_{m=1}^{\sigma} \left(\frac{\eta^{r_m}}{r_m!}\kappa(F_m)\right)^{\nu_m} \cdot \frac{\nu_q}{\frac{\eta^{r_q}}{r_q!}\kappa(F_q)} \quad .$$

$$\cdot\left(\sum_{j=1}^{i-1} \gamma_{ij}\frac{\psi_j(F_q)}{(r_q-1)!} + \gamma\,\frac{\psi_i(F_q)}{(r_q-1)!}\right)\Bigg\}\left[F_1^{\nu_1}\cdots F_\sigma^{\nu_\sigma}\,\frac{d^\nu f}{dy^\nu}\right]_n,$$

where

$$\nu = \sum_{i=1}^{\sigma} \nu_i$$

so

$$\psi_i(F) = (\bar{r}-1)!\,\prod_{m=1}^{\sigma}\frac{1}{\nu_m!}\left(\frac{1}{r_m!}\right)^{\nu_m}\left\{\sum_{m=1}^{\sigma}\left(\sum_{j=1}^{i-1}\alpha_{ij}r_m\psi_j(F_m)\right)^{\nu_m} +\right.$$

$$\left. + \prod_{m=1}^{\sigma}(\eta^{r_m}\kappa(F_m))^{\nu_m}\sum_{q=1}^{\sigma}\frac{\nu_q r_q}{\eta^{r_q}\kappa(F_q)}\left(\sum_{j=1}^{i-1}\gamma_{ij}\psi_j(F_q)+\gamma\psi_i(F_q)\right)\right\}.$$

We now can obtain the following result.

THEOREM 2.3.3. *If the conditions of lemma* 2.3.1 *are fulfilled, the approximate solution of* (2.3.1) *has the following expansion:*

$$y_{n+1} = y_n + \sum_{r=1}^{\infty}\frac{h^r}{r!}\sum_{\text{ord } F=r}\phi(F)[F]_n, \tag{2.3.8}$$

where

$$\phi(F) = r\sum_{i=1}^{s}\mu_i\psi_i(F),$$ *where* $\psi_i(F)$ *is given by* (2.3.6).

PROOF. When we substitute (2.3.3) in (2.3.2.b) we get:

$$y_{n+1} = y_n + h\sum_{i=1}^{s}\mu_i k_i = y_n + \sum_{r=1}^{\infty}\frac{h^r}{r!}\sum_{i=1}^{s}\mu_i\, r\, K_{i,r-1}$$

with lemma 2.3.2 we can write

$$y_{n+1} = y_n + \sum_{r=1}^{\infty}\frac{h^r}{r!}\sum_{i=1}^{s}\mu_i\, r\sum_{\text{ord } F=r}\psi_i(F)[F]_n$$

which is identical to (2.3.8).

COROLLARY 2.3.4. *To each elementary differential* F *corresponds an elementary* *weight* $\phi = \phi(F)$ *that is defined by:*

(2.3.9)

if order F is 1: $\phi(f) = \sum_{i=1}^{s} \mu_i$

if order F is r and $F = \{F_1^{\nu_1} \ldots F_\sigma^{\nu_\sigma}\}$ with F_i all distinct for $i = 1,\ldots,\sigma$:

$$\phi(F) = \sum_{i=1}^{s} \mu_i \Bigg\{ r! \prod_{m=1}^{\sigma} \frac{1}{\nu_m!} \left(\frac{1}{r_m!}\right)^{\nu_m} \Bigg\{ \prod_{m=1}^{\sigma} \Big(\sum_{j=1}^{i-1} \alpha_{ij}\, r_m\, \psi_j(F_m)\Big)^{\nu_m} +$$

$$\prod_{m=1}^{\sigma} \left(\eta^{r_m} \kappa(F_m)\right)^{\nu_m} \sum_{q=1}^{\sigma} \frac{\nu_q r_q}{\eta^{r_q} \kappa(F_q)} \left(\sum_{j=1}^{i-1} \gamma_{ij}\, \psi_j(F_q) + \gamma \psi_i(F_q) \right) \Bigg\} \Bigg\}$$

where $\psi_j(F)$ is given by (2.3.6) and $\kappa(F)$ by (2.1.1).

2.4. Taylor expansion of $\vec{y}_{n+1}$

Consider the system of ordinary differential equations:

$$\frac{d\vec{y}}{dx} = \vec{f}(\vec{y}), \quad x > x_n, \quad \vec{y}(x_n) = \vec{y}_n, \tag{2.4.1}$$

where

$$\vec{y} = (y_1,\ldots,y_N)^T, \quad \vec{f} = (f_1,\ldots,f_N)^T \text{ and } \vec{y}_n = (y_{n,1},\ldots,y_{n,N})^T.$$

In this section we will derive in an analogous way as in section 2.3, an expansion similar to (2.3.8) of the approximate solution $\vec{y}_{n+1}$ of (2.4.1) that is obtained by the s-stage RKR-method:

$$\begin{cases} \left[I - \gamma h \dfrac{\partial \vec{f}}{\partial \vec{y}}(\vec{y}_{n+\eta}) \right] \vec{k}_i = \vec{f}\Big(\vec{y}_n + h \sum\limits_{j=1}^{i-1} \alpha_{ij} \vec{k}_j\Big) + h \dfrac{\partial \vec{f}}{\partial \vec{y}}(\vec{y}_{n+\eta}) \sum\limits_{j=1}^{i-1} \gamma_{ij} \vec{k}_j \quad i=1,\ldots,s \\[2ex] \vec{y}_{n+1} = \vec{y}_n + h \sum\limits_{i=1}^{s} \mu_i \vec{k}_i, \end{cases} \tag{2.4.2}$$

where $\dfrac{\partial \vec{f}}{\partial \vec{y}}$ denotes the Jacobian matrix.

To simplify the derivation we will adopt from WOLFBRANDT [6] the following definition for vector functions $\vec{v}_i(\vec{y})$:

$$\vec{v}_1\vec{v}_2\cdots\vec{v}_k\frac{\partial^k}{\partial\vec{y}^k} = \sum_{j_1=1}^{N}\sum_{j_2=1}^{N}\cdots\sum_{j_k=1}^{N} v_{1j_1}v_{2j_2}\cdots v_{kj_k}\frac{\partial^k}{\partial y_{j_1}\cdots\partial y_{j_k}} .$$

In order to obtain a similarity with (2.3.2.a) we write for the ν-th component of $\vec{k}_i$:

$$k_i^{(\nu)} = [1-\gamma h\frac{\partial f_\nu}{\partial y_\nu}(\vec{y}_{n+\eta})]^{-1} \cdot$$

(2.4.3)

$$\{f_\nu(\vec{y}_n + h\sum_{j=1}^{i-1}\alpha_{ij}\vec{k}_j) + h\sum_{\ell=1}^{N}\frac{\partial f_\nu}{\partial y_\ell}(\vec{y}_{n+\eta})\sum_{j=1}^{i-1}\gamma_{ij}k_j^{(\ell)} +$$

$$+ \gamma h\sum_{\substack{\ell=1\\ \ell\neq\nu}}^{N}\frac{\partial f_\nu}{\partial y_\ell}(\vec{y}_{n+\eta})k_i^{(\ell)}\}.$$

We now proceed as in section 2.3.

Expand $\vec{k}_i$ in a power series

(2.4.4) $$\vec{k}_i = \sum_{r=0}^{\infty}\frac{h^r}{r!}\vec{K}_{i,r}, \qquad \text{where } \vec{K}_{i,r} = (K_{i,r}^{(1)},\ldots,K_{i,r}^{(N)})^T.$$

The analogous result of lemma 2.3.1 is:

<u>LEMMA 2.4.1</u>. *Let $\vec{f} = \vec{f}(\vec{y})$ be analytic and let $\vec{y}_{n+\eta}$ have an expansion of the form*

$$\vec{y}_{n+\eta} = \vec{y}_n + \sum_{r=1}^{\infty} h^r\vec{z}_r , \qquad \textit{where } \vec{z}_r = \frac{\eta^r}{r!}[D^{r-1}\vec{f}]_n .$$

Then the recurrence relation for the ν-th component of $\vec{K}_{i,r}$ is:

$$K_{i,0}^{(\nu)} = [f_\nu]_n$$

(2.4.5)

$$K_{i,r}^{(\nu)} = \sum_{k=1}^{r} \frac{r!}{k!} \sum_{r_1+\ldots+r_k=r} \left(\prod_{m=1}^{k} \sum_{j=1}^{i-1} \alpha_{ij} \frac{\vec{K}_{j,r_m-1}}{(r_m-1)!} \right) \left[\frac{\partial^k f_\nu}{\partial \vec{y}^k} \right]_n +$$

$$r \sum_{\ell=1}^{N} \left(\sum_{j=1}^{i-1} \gamma_{ij} K_{j,r-1}^{(\ell)} + \gamma\, K_{i,r-1}^{(\ell)} \right) \left[\frac{\partial f_\nu}{\partial y_\ell} \right]_n +$$

$$\sum_{\ell=1}^{N} \sum_{q=1}^{r-1} \sum_{k=1}^{q} \frac{r!}{k!} \sum_{r_1+\ldots+r_k=q} \left(\prod_{m=1}^{k} \vec{z}_{r_m} \right) \cdot$$

$$\cdot \left(\sum_{j=1}^{i-1} \gamma_{ij} \frac{K_{j,r-q-1}^{(\ell)}}{(r-q-1)!} + \gamma \frac{K_{i,r-q-1}^{(\ell)}}{(r-q-1)!} \right) \left[\frac{\partial^k}{\partial \vec{y}^k} \left(\frac{\partial f_\nu}{\partial y_\ell} \right) \right]_n , \qquad \nu = 1,2,\ldots,N.$$

<u>PROOF</u>. The proof of $K_{i,0}^{(\nu)} = [f_\nu]_n$ for $\nu = 1,2,\ldots,N$ is trivial.

Following the approach described in the proof of lemma 2.3.1 we find:

$$h \sum_{j=1}^{i-1} \gamma_{ij} k_j^{(\ell)} = \sum_{r=1}^{\infty} h^r \sum_{j=1}^{i-1} \gamma_{ij} \frac{K_{j,r-1}^{(\ell)}}{(r-1)!} \underset{=}{\text{not.}} \sum_{r=1}^{\infty} h^r c_{i,r}^{(\ell)}$$

$$\vec{y}_n + h \sum_{j=1}^{i-1} \alpha_{ij} \vec{k}_j = \vec{y}_n + \sum_{r=1}^{\infty} h^r \sum_{j=1}^{i-1} \alpha_{ij} \frac{\vec{K}_{j,r-1}}{(r-1)!} \underset{=}{\text{not.}} \sum_{r=1}^{\infty} h^r \vec{a}_{i,r}$$

Using Taylor's theorem for multiple variables and the multinomial theorem we obtain the powerseries for:

$$f_\nu(\vec{y}_n + h \sum_{j=1}^{i-1} \alpha_{ij} \vec{k}_j) = [f_\nu]_n + \sum_{r=1}^{\infty} h^r \sum_{k=1}^{r} \frac{1}{k!} \sum_{r_1+\ldots+r_k=r}$$

$$\left(\prod_{m=1}^{k} \vec{a}_{i,r_m} \right) \left[\frac{\partial^k f_\nu}{\partial \vec{y}^k} \right]_n$$

and for

$$\frac{\partial f_\nu}{\partial y_\ell}(\vec{y}_{n+\eta}) = \left[\frac{\partial f_\nu}{\partial y_\ell}\right]_n + \sum_{r=1}^{\infty} h^r \sum_{k=1}^{r} \frac{1}{k!} \sum_{r_1+\ldots+r_k=r} \left(\prod_{m=1}^{k} \vec{z}_{r_m}\right)\left[\frac{\partial^k}{\partial \vec{y}^k}\left(\frac{\partial f_\nu}{\partial y_\ell}\right)\right]_n .$$

Let

$$A = 1 - \gamma h \frac{\partial f_\nu}{\partial y_\nu}(\vec{y}_{n+\eta})$$
$$= 1 - \gamma h\left[\frac{\partial f_\nu}{\partial y_\nu}\right]_n - \gamma \sum_{r=2}^{\infty} h^r \sum_{k=1}^{r-1} \frac{1}{k!} \sum_{r_1+\ldots+r_k=r-1} \left(\prod_{m=1}^{k} \vec{z}_{r_m}\right)\left[\frac{\partial^k}{\partial \vec{y}^k}\left(\frac{\partial f_\nu}{\partial y_\nu}\right)\right]_n$$

and

$$B = f_\nu(\vec{y}_n + h\sum_{j=1}^{i-1} \alpha_{ij}\vec{k}_j) + h\sum_{\ell=1}^{N} \frac{\partial f_\nu}{\partial y_\ell}(\vec{y}_{n+\eta})\sum_{j=1}^{i-1} \gamma_{ij}k_j^{(\ell)} +$$
$$\gamma h \sum_{\substack{\ell=1\\ \ell\neq\nu}}^{N} \frac{\partial f_\nu}{\partial y_\ell}(\vec{y}_{n+\eta})k_i^{(\ell)}$$
$$= [f_\nu]_n + \sum_{r=1}^{\infty} h^r\left\{\sum_{k=1}^{r} \frac{1}{k!} \sum_{r_1+\ldots+r_k=r} \left(\prod_{m=1}^{k} \vec{a}_{i,r_m}\right)\left[\frac{\partial^k f_\nu}{\partial \vec{y}^k}\right]_n +\right.$$
$$\sum_{\ell=1}^{N}\left(\left[\frac{\partial f_\nu}{\partial y_\ell}\right]_n c_{i,r}^{(\ell)} + \sum_{q=1}^{r-1}\left(\sum_{k=1}^{q} \frac{1}{k!} \sum_{r_1+\ldots+r_k=q} \left(\prod_{m=1}^{k} \vec{z}_{r_m}\right)\cdot\right.\right.$$
$$\left.\left.\cdot\left[\frac{\partial^k}{\partial \vec{y}^k}\left(\frac{\partial f_\nu}{\partial y_\ell}\right)\right]_n\right)\left(c_{i,r-q}^{(\ell)}\right)\right) + \gamma \sum_{\substack{\ell=1\\ \ell\neq\nu}}^{N}\left(\left[\frac{\partial f_\nu}{\partial y_\ell}\right]_n \frac{K_{i,r-1}^{(\ell)}}{(r-1)!} +\right.$$
$$\left.\left.\sum_{q=1}^{r-1}\left(\sum_{k=1}^{q} \frac{1}{k!} \sum_{r_1+\ldots+r_k=q} \left(\prod_{m=1}^{k} \vec{z}_{r_m}\right)\left[\frac{\partial^k}{\partial \vec{y}^k}\left(\frac{\partial f_\nu}{\partial y_\ell}\right)\right]_n\right)\left(\frac{K_{i,r-q-1}^{(\ell)}}{(r-q-1)!}\right)\right)\right\}$$

Then we get for the right hand side of (2.4.3):

$$A^{-1}B = \sum_{r=0}^{\infty} h^{r} b_{r},$$

where

$$b_0 = [f_\nu]_n,$$

and

$$b_r = \sum_{k=1}^{r} \frac{1}{k!} \sum_{r_1+\dots+r_k=r} \left(\prod_{m=1}^{k} \vec{a}_{i,r_m}\right)\left[\frac{\partial^k f_\nu}{\partial \vec{y}^{\,k}}\right]_n +$$

$$\sum_{\ell=1}^{N}\bigg(\left[\frac{\partial f_\nu}{\partial y_\ell}\right]_n c_{i,r}^{(\ell)} + \sum_{q=1}^{r-1}\bigg(\sum_{q=1}^{q}\frac{1}{k!}\sum_{r_1+\dots+r_k=q}\left(\prod_{m=1}^{k}\vec{z}_{r_m}\right)\left[\frac{\partial^k}{\partial\vec{y}^{\,k}}\left(\frac{\partial f_\nu}{\partial y_\ell}\right)\right]_n\bigg)\cdot$$

$$\cdot\left(c_{i,r-q}^{(\ell)}\right)\bigg) + \gamma \sum_{\substack{\ell=1\\ \ell\neq\nu}}^{N}\bigg(\left[\frac{\partial f_\nu}{\partial y_\ell}\right]_n \frac{K_{i,r-1}^{(\ell)}}{(r-1)!} + \sum_{q=1}^{r-1}\bigg(\sum_{k=1}^{q}\frac{1}{k!}\sum_{r_1+\dots+r_k=q}$$

$$\left(\prod_{m=1}^{k}\vec{z}_{r_m}\right)\left[\frac{\partial^k}{\partial\vec{y}^{\,k}}\left(\frac{\partial f_\nu}{\partial y_\ell}\right)\right]_n\left(\frac{K_{i,r-q-1}^{(\ell)}}{(r-q-1)!}\right)\bigg)\bigg) +$$

$$\sum_{q=0}^{r-2} b_q \gamma \sum_{k=1}^{r-q-1}\frac{1}{k!}\sum_{r_1+\dots+r_k=r-q-1}\left(\prod_{m=1}^{k} \vec{z}_{r_m}\right)\left[\frac{\partial^k}{\partial\vec{y}^{\,k}}\left(\frac{\partial f_\nu}{\partial y_\nu}\right)\right]_n +$$

$$b_{r-1}\gamma\left[\frac{\partial f_\nu}{\partial y_\nu}\right]_n .$$

From (2.4.3) and (2.4.4) it follows that

$$\sum_{r=0}^{\infty} h_r \frac{K_{i,r}^{(\nu)}}{r!} = \sum_{r=0}^{\infty} h^r b_r$$

so

$$K_{i,r}^{(\nu)} = r!\,\bigg\{\sum_{k=1}^{r} \frac{1}{k!}\sum_{r_1+\dots+r_k=r}\left(\prod_{m=1}^{k}\sum_{j=1}^{i-1}\alpha_{ij}\frac{\vec{K}_{j,r_m-1}}{(r_m-1)!}\right)\left[\frac{\partial^k f_\nu}{\partial\vec{y}^{\,k}}\right]_n +$$

$$\sum_{\ell=1}^{N}\left(\sum_{j=1}^{i-1}\gamma_{ij}\frac{K_{j,r-1}^{(\ell)}}{(r-1)!}\left[\frac{\partial f_\nu}{\partial y_\ell}\right]_n\right. +$$

$$\sum_{q=1}^{r-1}\left(\sum_{k=1}^{q}\frac{1}{k!}\sum_{r_1+\ldots+r_k=q}\left(\prod_{m=1}^{k}\vec{z}_{r_m}\right)\left[\frac{\partial^k}{\partial\vec{y}^k}\left(\frac{\partial f_\nu}{\partial y_\ell}\right)\right]_n\right)\left(\sum_{j=1}^{i-1}\gamma_{ij}\frac{K_{j,r-q-1}^{(\ell)}}{(r-q-1)!}\right)\Bigg) +$$

$$\gamma\sum_{\substack{\ell=1\\ \ell\neq\nu}}^{N}\left(\left[\frac{\partial f_\nu}{\partial y_\ell}\right]_n\frac{K_{i,r-1}^{(\ell)}}{(r-1)!} + \sum_{q=1}^{r-1}\left(\sum_{k=1}^{q}\frac{1}{k!}\sum_{r_1+\ldots+r_k=q}\left(\prod_{m=1}^{k}\vec{z}_{r_m}\right)\cdot\right.\right.$$

$$\cdot\left[\frac{\partial^k}{\partial\vec{y}^k}\left(\frac{\partial f_\nu}{\partial y_\ell}\right)\right]_n\Bigg)\left(\frac{K_{i,r-q-1}^{(\ell)}}{(r-q-1)!}\right)\Bigg) +$$

$$\gamma\sum_{q=0}^{r-2}\frac{K_{i,q}^{(\nu)}}{q!}\sum_{k=1}^{r-q-1}\frac{1}{k!}\sum_{r_1+\ldots+r_k=r-q-1}\left(\prod_{m=1}^{k}\vec{z}_{r_m}\right)\left[\frac{\partial^k}{\partial\vec{y}^k}\left(\frac{\partial f_\nu}{\partial y_\nu}\right)\right]_n +$$

$$\gamma\frac{K_{i,r-1}^{(\nu)}}{(r-1)!}\left[\frac{\partial f_\nu}{\partial y_\nu}\right]_n$$

for $\nu = 1,2,\ldots,N$, which is equivalent to (2.4.5). □

The result of this lemma is identical to that of lemma 2.3.1 with vector functions instead of scalars.

That lemma 2.3.2, theorem 2.3.3 and corollary 2.3.4 also hold for systems of ordinary differential equations (when the scalars f, F, y and y_n are replaced by the vectors $\vec{f},\vec{F},\vec{y}$ and $\vec{y}_n$) can now be verified in the same way as in section 2.3.

2.5. Conditions for the coefficients.

In the preceding sections we have shown that the exact and the approximate solution of the initial value problem (2.4.1) at the point x_n+h can be expanded in powers of h about the point x_n

$$\vec{y}(x_n+h) = \vec{y}_n + \sum_{r=1}^{\infty}\frac{h^r}{r!}\sum_{\text{ord }\vec{F}=r}\kappa(\vec{F})[\vec{F}]_n,$$

where $\kappa(F)$ is given by (2.1.1) and

$$\vec{y}_{n+1} = \vec{y}_n + \sum_{r=1}^{\infty} \frac{h^r}{r!} \sum_{\text{ord } \vec{F}=r} \phi(\vec{F})[\vec{F}]_n,$$

where $\phi(\vec{F})$ is given by (2.3.9).

The two expressions agree up to terms in h^ρ if

(2.5.1) $\phi(\vec{F}) = \kappa(\vec{F})$ when $r \leq \rho$ and r is the order of $\vec{F}$

while the error is given by:

(2.5.2) $$\vec{y}_{n+1} - \vec{y}(x_n+h) = \sum_{r=\rho+1}^{\infty} \frac{h^r}{r!} \sum_{\text{ord } \vec{F}=r} (\phi(\vec{F})-\kappa(\vec{F}))[\vec{F}]_n$$

3. GENERATION OF THE ORDER CONDITIONS

3.1. Elementary differentials and trees

The generation of the order conditions is based on the fact that there is a one-to-one correspondence between the elementary differentials of $\vec{f}$ of order r and the rooted trees with r nodes (see HAIRER & WANNER [4], and BUTCHER [2]).

A rooted tree t, often simply called a tree, is defined as a connected graph without cycles with one unique specified node, the root.

The notation

$$t = [t_1,\ldots,t_m]$$

means that the trees $t_1,\ldots,t_m$ remain after the root of t and the adjacent arcs have been removed.

The tree consisting of only one node (the root) is denoted by τ.

The correspondence between the elementary differentials of $\vec{f}$ of order r and the set of trees with r nodes can be recursively defined by:

(i) $\vec{f}$ corresponds to τ

(ii) $\{\vec{F}\ldots\vec{F}_m\}$ corresponds to $[t_1,\ldots,t_m]$ if the elementary differentials $\vec{F}_i$, $i = 1,\ldots,m$, correspond to the trees t_i.

As an example we give for the elementary differentials up to order 4 the corresponding trees in their formal form and represented as a graph. For the formal notation of a tree we use similar conventions as for the elementary differentials (see section 2.1), e.g. $[[\tau,\tau,\tau]] = [_2\tau^3]_2$

$\vec{f}$	τ				
$\{\vec{f}\}$	$[\tau]$				
$\{\vec{f}^2\}$	$[\tau^2]$		$\{_2\vec{f}\}_2$	$[_2\tau]_2$	
$\{\vec{f}^3\}$	$[\tau^3]$		$\{\{\vec{f}\}\vec{f}\}$	$[[\tau],\tau]$	
$\{_2\vec{f}^2\}_2$	$[_2\tau^2]_2$		$\{_3\vec{f}\}_3$	$[_3\tau]_3$	

3.2. Outline of the computer program

To get the order conditions from equation (2.5.1) we wrote a computer program in ALGOL68 of which we will give a short outline. The program is based on a slightly changed version of a formula manipulation package written by DEKKER [3].

Suppose we wish to obtain the order conditions up to order $\bar{r}$. We then have to compute for each elementary differential $\vec{F}$ of order $r \le \bar{r}$ the value $\kappa(\vec{F})$ (2.1.1) and the polynomial $\psi_i(\vec{F})$ (2.3.6).

In view of the correspondence between the set of elementary differentials of $\vec{f}$ of order r and the set of trees with r nodes we can represent an elementary differential $\vec{F}$ by its corresponding tree. We therefore build up the set T of all trees with a number of nodes not exceeding $\bar{r}$. An element of this set will be denoted by $T_{r,k}$, where r is the number of nodes (the order) of the tree and k the number of the tree in the list of all trees of order r (the order list). To each tree a list of elements (subtrees) is linked. Each element contains the order of the subtree, the number of this subtree in its order list and the number of times this subtree occurs in the tree.

We now compute for each tree $T_{r,k}$, starting with $T_{1,1}$, an integer value

$K_{r,k}$ and a polynomial $\Psi^i_{r,k}$. For instance, if the tree $T_{r,k} = [T^{\nu_1}_{r_1,k_1},\dots,T^{\nu_\sigma}_{r_\sigma,k_\sigma}]$ corresponds with the elementary differential $\vec{F} = \{\vec{F}_1^{\nu_1}\dots\vec{F}_\sigma^{\nu_\sigma}\}$ then $K_{r,k} = \kappa(\vec{F})$ and $\Psi^i_{r,k} = \psi_i(\vec{F})$. For each subtree T_{r_j,k_j} the numbers r_j, k_j and ν_j have been stored in the list that is linked to $T_{r,k}$. Moreover $\kappa(\vec{F}_j)$, (K_{r_j,k_j}), and $\psi_i(\vec{F}_j),(\Psi^i_{r_j,k_j})$, have already been computed for the tree T_{r_j,k_j} that corresponds with $\vec{F}_j$.

In this way we can build up the set K consisting of integer values and the set Ψ consisting of polynomials. We next equate for r from 1 up to $\bar{r}$ and for all possible k

$$r \sum_{i=1}^{s} \mu_i \Psi^i_{r,k} = K_{r,k}.$$

From these relations we then obtain, after some manipulation, the desired order conditions.

In table 1 we give the order conditions up to and including order 6. The third column contains the number by which the equation has been divided. Hence to get the real error constant $\phi(\vec{F}) - \kappa(\vec{F})$ in (2.5.2), one has to multiply the difference between the left hand side and the right hand side of the order equation with this number. Further we used the following abbreviations in the table:

$$\beta_{ij} = \alpha_{ij} + \gamma_{ij}$$

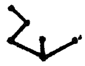
$$\alpha_i = \sum_{j=1}^{i-1} \alpha_{ij} \qquad \beta_i = \sum_{j=1}^{i-1} \beta_{ij}$$

$$\alpha_{ij} = \gamma_{ij} = 0 \quad \text{for } i \le j.$$

Table 1. Order conditions for $r \le 6$

1		1	$\Sigma\mu_i = 1$
2		2	$\Sigma\mu_i\beta_i = \frac{1}{2} - \gamma$

3		3	$\Sigma\mu_i\alpha_i^2 = \frac{1}{3} - \eta(1-2\Sigma\mu_i\alpha_i)$
		6	$\Sigma\mu_i\beta_{ij}\beta_j = \frac{1}{6} - \gamma + \gamma^2$
4		4	$\Sigma\mu_i\alpha_i^3 = \frac{1}{4} - \eta^2(\frac{3}{2} - 3\Sigma\mu_i\alpha_i)$
		24	$\Sigma\mu_i\alpha_i\alpha_{ij}\beta_j = \frac{1}{8} - \frac{1}{3}\gamma - \eta(\frac{1}{6} - \Sigma\mu_i\alpha_{ij}\beta_j - \gamma(1 - \Sigma\mu_i\alpha_i)) - \eta^2(\frac{1}{4} - \frac{1}{2}\Sigma\mu_i\alpha_i)$
		12	$\Sigma\mu_i\beta_{ij}\alpha_j^2 = \frac{1}{12} - \frac{1}{3}\gamma - \eta(\frac{1}{3} - 2\Sigma\mu_i\beta_{ij}\alpha_j - \gamma)$
		24	$\Sigma\mu_i\beta_{ij}\beta_{jk}\beta_k = \frac{1}{24} - \frac{1}{2}\gamma + \frac{3}{2}\gamma^2 - \gamma^3$
5		5	$\Sigma\mu_i\alpha_i^4 = \frac{1}{5} - \eta^3(2 - 4\Sigma\mu_i\alpha_i)$
		60	$\Sigma\mu_i\alpha_i^2\alpha_{ij}\beta_j = \frac{1}{10} - \frac{1}{4}\gamma - \eta^2(\frac{1}{6} - \Sigma\mu_i\alpha_{ij}\beta_j - \gamma(\frac{3}{2} - 2\Sigma\mu_i\alpha_i)) - \eta^3(\frac{1}{2} - \Sigma\mu_i\alpha_i)$
		60	$\Sigma\mu_i\alpha_{ij}\beta_j\alpha_{ik}\beta_k = \frac{1}{20} - \frac{1}{4}\gamma + \frac{1}{3}\gamma^2 + \eta\gamma(\frac{1}{3} - 2\Sigma\mu_i\alpha_{ij}\beta_j - \gamma) - \eta^2(\frac{1}{6} - \Sigma\mu_i\alpha_{ij}\beta_j - \frac{1}{2}\gamma)$
		60	$\Sigma\mu_i\alpha_i\alpha_{ij}\alpha_j^2 = \frac{1}{15} - \eta(\frac{1}{3} - \Sigma\mu_i\alpha_{ij}\alpha_j^2 - 2\Sigma\mu_i\alpha_i\alpha_{ij}\alpha_j) + \eta^2(\frac{1}{3} - 2\Sigma\mu_i\alpha_{ij}\alpha_j) + \eta^3(\frac{1}{3} - \frac{2}{3}\Sigma\mu_i\alpha_i)$
		120	$\Sigma\mu_i\alpha_i\alpha_{ij}\beta_{jk}\beta_k = \frac{1}{30} - \frac{1}{4}\gamma + \frac{1}{3}\gamma^2 - \eta(\frac{1}{24} - \Sigma\mu_i\alpha_{ij}\beta_{jk}\beta_k - \frac{1}{3}\gamma + \gamma^2(1-\Sigma\mu_i\alpha_i)) + \eta^2\gamma(\frac{1}{2} - \Sigma\mu_i\alpha_i) - \eta^3(\frac{1}{12} - \frac{1}{6}\Sigma\mu_i\alpha_i)$
		20	$\Sigma\mu_i\beta_{ij}\alpha_j^3 = \frac{1}{20} - \frac{1}{4}\gamma - \eta^2(\frac{1}{2} - 3\Sigma\mu_i\beta_{ij}\alpha_j - \frac{3}{2}\gamma)$
		120	$\Sigma\mu_i\beta_{ij}\alpha_j\alpha_{jk}\beta_k = \frac{1}{40} - \frac{5}{24}\gamma + \frac{1}{3}\gamma^2 - \eta(\frac{1}{24} - \Sigma\mu_i\beta_{ij}\alpha_{jk}\beta_k - \gamma(\frac{1}{2} - \Sigma\mu_i\beta_{ij}\alpha_j) + \gamma^2) - \eta^2(\frac{1}{12} - \frac{1}{2}\Sigma\mu_i\beta_{ij}\alpha_j - \frac{1}{4}\gamma)$
		60	$\Sigma\mu_i\beta_{ij}\beta_{jk}\alpha_k^2 = \frac{1}{60} - \frac{1}{6}\gamma + \frac{1}{3}\gamma^2 - \eta(\frac{1}{12} - 2\Sigma\mu_i\beta_{ij}\beta_{jk}\alpha_k - \frac{2}{3}\gamma + \gamma^2)$
		120	$\Sigma\mu_i\beta_{ij}\beta_{jk}\beta_{k\ell}\beta_\ell = \frac{1}{120} - \frac{1}{6}\gamma + \gamma^2 - 2\gamma^3 + \gamma^4$
6		6	$\Sigma\mu_i\alpha_i^5 = \frac{1}{6} - \eta^4(\frac{5}{2} - 5\Sigma\mu_i\alpha_i)$
		120	$\Sigma\mu_i\alpha_i^3\alpha_{ij}\beta_j = \frac{1}{12} - \frac{1}{5}\gamma - \eta^3(\frac{1}{6} - \Sigma\mu_i\alpha_{ij}\beta_j - \gamma(2 - 3\Sigma\mu_i\alpha_i)) - \eta^4(\frac{3}{4} - \frac{3}{2}\Sigma\mu_i\alpha_i)$

6		360	$\Sigma\mu_i\alpha_i\alpha_{ij}\beta_j\alpha_{ik}\beta_k = \frac{1}{24}-\frac{1}{5}\gamma+\frac{1}{4}\gamma^2+\eta^2\gamma(\frac{1}{3}-2\Sigma\mu_i\alpha_{ij}\beta_j - \gamma(\frac{3}{2}-\Sigma\mu_i\alpha_i)) - \eta^3(\frac{1}{6}-\Sigma\mu_i\alpha_{ij}\beta_j-\gamma(1-\Sigma\mu_i\alpha_i)) - \eta^4(\frac{1}{8}-\frac{1}{4}\Sigma\mu_i\alpha_i)$
		180	$\Sigma\mu_i\alpha_i^2\alpha_{ij}\alpha_j^2 = \frac{1}{18}-\eta(\frac{1}{5}-2\Sigma\mu_i\alpha_i^2\alpha_{ij}\alpha_j)-\eta^2(\frac{1}{12}-\Sigma\mu_i\alpha_{ij}\alpha_j^2)+\eta^3(\frac{1}{3}-2\Sigma\mu_i\alpha_{ij}\alpha_j)+\eta^4(\frac{2}{3}-\frac{4}{3}\Sigma\mu_i\alpha_i)$
		360	$\Sigma\mu_i\alpha_i^2\alpha_{ij}\beta_{jk}\beta_k = \frac{1}{36}-\frac{1}{5}\gamma+\frac{1}{4}\gamma^2-\eta^2(\frac{1}{24}-\Sigma\mu_i\alpha_{ij}\beta_{jk}\beta_k-\frac{1}{3}\gamma+\gamma^2(\frac{3}{2}-2\Sigma\mu_i\alpha_i))+\eta^3\gamma(1-2\Sigma\mu_i\alpha_i)-\eta^4(\frac{1}{6}-\frac{1}{3}\Sigma\mu_i\alpha_i)$
		360	$\Sigma\mu_i\alpha_{ij}\alpha_j^2\alpha_{ik}\beta_k = \frac{1}{36}-\frac{1}{15}\gamma-\eta(\frac{1}{10}-2\Sigma\mu_i\alpha_{ij}\alpha_j\alpha_{ik}\beta_k-\gamma(\frac{1}{3}-\Sigma\mu_i\alpha_{ij}\alpha_j^2)) - \eta^2(\frac{1}{24}-\frac{1}{2}\Sigma\mu_i\alpha_{ij}\alpha_j^2+\gamma(\frac{1}{3}-2\Sigma\mu_i\alpha_{ij}\alpha_j)) + \eta^3(\frac{5}{18}-\Sigma\mu_i\alpha_{ij}\alpha_j-\frac{2}{3}\Sigma\mu_i\alpha_{ij}\beta_j-\frac{1}{3}\gamma)$
		720	$\Sigma\mu_i\alpha_{ij}\beta_{jk}\beta_k\alpha_{i\ell}\beta_\ell = \frac{1}{72}-\frac{2}{15}\gamma+\frac{3}{8}\gamma^2-\frac{1}{3}\gamma^3+\eta\gamma(\frac{1}{24}-\Sigma\mu_i\alpha_{ij}\beta_{jk}\beta_k - \gamma(\frac{1}{2}-\Sigma\mu_i\alpha_{ij}\beta_j)+\gamma^2)-\eta^2(\frac{1}{48}-\frac{1}{2}\Sigma\mu_i\alpha_{ij}\beta_{jk}\beta_k - \gamma(\frac{1}{3}-\Sigma\mu_i\alpha_{ij}\beta_j)+\frac{3}{4}\gamma^2)-\eta^3(\frac{1}{36}-\frac{1}{6}\Sigma\mu_i\alpha_{ij}\beta_j-\frac{1}{12}\gamma)$
		120	$\Sigma\mu_i\alpha_i\alpha_{ij}\alpha_j^3 = \frac{1}{24}-\eta(\frac{1}{20}-\Sigma\mu_i\alpha_{ij}\alpha_j^3)-\eta^2(\frac{3}{8}-3\Sigma\mu_i\alpha_i\alpha_{ij}\alpha_j)+\eta^3(\frac{1}{2}-3\Sigma\mu_i\alpha_{ij}\alpha_j)+\eta^4(\frac{5}{8}-\frac{5}{4}\Sigma\mu_i\alpha_i)$
		720	$\Sigma\mu_i\alpha_i\alpha_{ij}\alpha_j\alpha_{jk}\beta_k = \frac{1}{48}-\frac{1}{15}\gamma-\eta(\frac{7}{120}-\Sigma\mu_i\alpha_{ij}\alpha_j\alpha_{jk}\beta_k-\Sigma\mu_i\alpha_i\alpha_{ij}\alpha_{jk}\beta_k - \gamma(\frac{1}{3}-\Sigma\mu_i\alpha_i\alpha_{ij}\alpha_j))-\eta^2(\frac{1}{48}+\Sigma\mu_i\alpha_{ij}\alpha_{jk}\beta_k - \frac{1}{2}\Sigma\mu_i\alpha_i\alpha_{ij}\alpha_j+\gamma(\frac{1}{3}-\Sigma\mu_i\alpha_{ij}\alpha_j)) + \eta^3(\frac{1}{12}-\frac{1}{2}\Sigma\mu_i\alpha_{ij}\alpha_j-\gamma(\frac{1}{3}-\frac{2}{3}\Sigma\mu_i\alpha_i)) + \eta^4(\frac{7}{48}-\frac{7}{24}\Sigma\mu_i\alpha_i)$
		360	$\Sigma\mu_i\alpha_i\alpha_{ij}\beta_{jk}\alpha_k^2 = \frac{1}{72}-\frac{1}{15}\gamma-\eta(\frac{1}{12}-\Sigma\mu_i\alpha_{ij}\beta_{jk}\alpha_k^2-2\Sigma\mu_i\alpha_i\alpha_{ij}\beta_{jk}\alpha_k - \frac{1}{3}\gamma)+\eta^2(\frac{1}{12}-2\Sigma\mu_i\alpha_{ij}\beta_{jk}\alpha_k-\frac{1}{3}\gamma) - \eta^3\gamma(\frac{1}{3}-\frac{2}{3}\Sigma\mu_i\alpha_i)+\eta^4(\frac{1}{8}-\frac{1}{4}\Sigma\mu_i\alpha_i)$
		720	$\Sigma\mu_i\alpha_i\alpha_{ij}\beta_{jk}\beta_{k\ell}\beta_\ell = \frac{1}{144}-\frac{1}{10}\gamma+\frac{3}{8}\gamma^2-\frac{1}{3}\gamma^3-\eta(\frac{1}{120}-\Sigma\mu_i\alpha_{ij}\beta_{jk}\beta_{k\ell}\beta_\ell - \frac{1}{8}\gamma+\frac{1}{2}\gamma^2-\gamma^3(1-\Sigma\mu_i\alpha_i))-\eta^2\gamma^2(\frac{3}{4}-\frac{3}{2}\Sigma\mu_i\alpha_i)+\eta^3\gamma(\frac{1}{4}-\frac{1}{2}\Sigma\mu_i\alpha_i)-\eta^4(\frac{1}{48}-\frac{1}{24}\Sigma\mu_i\alpha_i)$

6		30	$\Sigma\mu_i\beta_{ij}\alpha_j^4 = \frac{1}{30}-\frac{1}{5}\gamma-\eta^3(\frac{2}{3}-4\Sigma\mu_i\beta_{ij}\alpha_j-2\gamma)$
		360	$\Sigma\mu_i\beta_{ij}\alpha_j^2\alpha_{jk}\beta_k = \frac{1}{60}-\frac{3}{20}\gamma+\frac{1}{4}\gamma^2-\eta^2(\frac{1}{24}-\Sigma\mu_i\beta_{ij}\alpha_{jk}\beta_k - \gamma(\frac{2}{3}-2\Sigma\mu_i\beta_{ij}\alpha_j)+\frac{3}{2}\gamma^2) - \eta^3(\frac{1}{6}-\Sigma\mu_i\beta_{ij}\alpha_j-\frac{1}{2}\gamma)$
		360	$\Sigma\mu_i\beta_{ij}\alpha_{jk}\beta_k\alpha_{j\ell}\beta_\ell = \frac{1}{120}-\frac{1}{10}\gamma+\frac{1}{3}\gamma^2-\frac{1}{3}\gamma^3+\eta\gamma(\frac{1}{12}-2\Sigma\mu_i\beta_{ij}\alpha_{jk}\beta_k - \frac{2}{3}\gamma+\gamma^2)-\eta^2(\frac{1}{24}-\Sigma\mu_i\beta_{ij}\alpha_{jk}\beta_k-\frac{1}{3}\gamma+\frac{1}{2}\gamma^2)$
		360	$\Sigma\mu_i\beta_{ij}\alpha_j\alpha_{jk}\alpha_k^2 = \frac{1}{90}-\frac{1}{15}\gamma-\eta(\frac{1}{15}-\Sigma\mu_i\beta_{ij}\alpha_{jk}\alpha_k^2-2\Sigma\mu_i\beta_{ij}\alpha_j\alpha_{jk}\alpha_k - \frac{1}{3}\gamma)+\eta^2(\frac{1}{12}-2\Sigma\mu_i\beta_{ij}\alpha_{jk}\alpha_k-\frac{1}{3}\gamma)+ \eta^3(\frac{1}{9}-\frac{2}{3}\Sigma\mu_i\beta_{ij}\alpha_j-\frac{1}{3}\gamma)$
		720	$\Sigma\mu_i\beta_{ij}\alpha_j\alpha_{jk}\beta_{k\ell}\beta_\ell = \frac{1}{180}-\frac{1}{12}\gamma+\frac{1}{3}\gamma^2-\frac{1}{3}\gamma^3-\eta(\frac{1}{120}-\Sigma\mu_i\beta_{ij}\alpha_{jk}\beta_{k\ell}\beta_\ell - \frac{1}{8}\gamma+\gamma^2(\frac{2}{3}-\Sigma\mu_i\beta_{ij}\alpha_j)-\gamma^3) + \eta^2\gamma(\frac{1}{6}-\Sigma\mu_i\beta_{ij}\alpha_j-\frac{1}{2}\gamma) - \eta^3(\frac{1}{36}-\frac{1}{6}\Sigma\mu_i\beta_{ij}\alpha_j-\frac{1}{12}\gamma)$
		120	$\Sigma\mu_i\beta_{ij}\beta_{jk}\alpha_k^3 = \frac{1}{120}-\frac{1}{10}\gamma+\frac{1}{4}\gamma^2-\eta^2(\frac{1}{8}-3\Sigma\mu_i\beta_{ij}\beta_{jk}\alpha_k-\gamma+\frac{3}{2}\gamma^2)$
		720	$\Sigma\mu_i\beta_{ij}\beta_{jk}\alpha_k\alpha_{k\ell}\beta_\ell = \frac{1}{240}-\frac{1}{15}\gamma+\frac{7}{24}\gamma^2-\frac{1}{3}\gamma^3-\eta(\frac{1}{120}-\Sigma\mu_i\beta_{ij}\beta_{jk}\alpha_{k\ell}\beta_\ell - \gamma(\frac{1}{6}-\Sigma\mu_i\beta_{ij}\beta_{jk}\alpha_k)+\frac{5}{6}\gamma^2-\gamma^3) - \eta^2(\frac{1}{48}-\frac{1}{2}\Sigma\mu_i\beta_{ij}\beta_{jk}\alpha_k-\frac{1}{6}\gamma+\frac{1}{4}\gamma^2)$
		360	$\Sigma\mu_i\beta_{ij}\beta_{jk}\beta_{k\ell}\alpha_\ell^2 = \frac{1}{360}-\frac{1}{20}\gamma+\frac{1}{4}\gamma^2-\frac{1}{3}\gamma^3-\eta(\frac{1}{60}-2\Sigma\mu_i\beta_{ij}\beta_{jk}\beta_{k\ell}\alpha_\ell - \frac{1}{4}\gamma+\gamma^2-\gamma^3)$
		720	$\Sigma\mu_i\beta_{ij}\beta_{jk}\beta_{k\ell}\beta_{\ell m}\beta_m = \frac{1}{720}-\frac{1}{24}\gamma+\frac{5}{12}\gamma^2-\frac{5}{3}\gamma^3+\frac{5}{2}\gamma^4-\gamma^5$

REMARK. If η is a non-positive real value the relation

$$z_r = \frac{\eta^r}{r!}\left[D^{r-1}f\right]_n$$

is in general only satisfied for $r \le p-2$, where p denotes the order of consistency.

This restriction has no influence on the resulting order conditions. However, the formula for the error (2.5.2) is in that case not correct.

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