

## Fully Implicit Runge-Kutta Methods

Hint:

A numerical integration rule has *order*  $p$  if it has *degree*  $p - 1$ ; cf. § 2.3(a), i.e. is exact for all polynomials  $\psi \in \Pi_{p-1}$  (!).

We consider two types of differential systems with sufficiently smooth data, namely the general nonlinear system and the linear system:

$$y'(t) = f(t, y(t)) \in \mathbb{R}^m, \quad (1)$$

$$y'(t) = B(t)y(t) + c(t) \in \mathbb{R}^m, B(t) \in \mathbb{R}^m_m. \quad (2)$$

To a  $r$ -stage Runge-Kutta method (RKM) with BUTCHER matrix  $[A, b, c]$ , there are the integration rules for the interior equations and exterior equation associated:

$$\int_0^{\gamma_i} f(t) dt \simeq \sum_{j=1}^r a_{ij} f(\gamma_j), \quad i = 1 : r, \quad A = [a_{ij}]_{i,j=1}^r \quad (3)$$

$$\int_0^1 f(t) dt \simeq \sum_{j=1}^r \beta_j f(\gamma_j). \quad (4)$$

Let  $Z(t)$  be the solution of the implicit system of interior equations,

$$Z(t) = e \times y(t) + \tau(A \times I)F(t, Z(t)),$$

then

$$d(t, y, \tau) = \frac{y(t + \tau) - y(t)}{\tau} - (b \times I)^T F(t, Z(t))$$

is the *discretization error* where

$$F(t, Z(t)) = [f(t_i, z_i(t_i))]_{i=1}^r \in \mathbb{R}^{r \cdot n}, \quad t_i = t + \gamma_i \tau.$$

**Notations:** cf. [Dekker]

$\mathcal{A}(\varrho)$	$\iff$	RKM has order $\varrho$	$\iff$	$d(t, y, \tau) = \mathcal{O}(\tau^\varrho)$	
$\mathcal{B}(\varrho)$	$\iff$	$\sum_{i=1}^r \beta_i \gamma_i^{k-1} = \frac{1}{k},$		$k = 1 : \varrho$	
$\mathcal{C}(\varrho)$	$\iff$	$\sum_{j=1}^r a_{ij} \gamma_j^{k-1} = \frac{1}{k} \gamma_i^k,$		$i = 1 : r, k = 1 : \varrho$	
$\mathcal{D}(\varrho)$	$\iff$	$\sum_{i=1}^r \beta_i \gamma_i^{k-1} a_{ij} = \frac{1}{k} \beta_j (1 - \gamma_j^k),$		$j = 1 : r, k = 1 : \varrho$	
$\mathcal{E}(\varrho, \eta)$	$\iff$	$\sum_{i,j=1}^r \beta_i \gamma_i^{\ell-1} a_{ij} \gamma_j^{k-1} = \frac{1}{k(\ell+k)},$		$\ell = 1 : \varrho, k = 1 : \eta$	(5)

Let

$$\boxed{\begin{aligned} b &= [\beta_1, \beta_2, \dots, \beta_r]^T \in \mathbb{R}^r, & c &= [\gamma_1, \gamma_2, \dots, \gamma_r]^T \in \mathbb{R}^r, & C &= \text{diag}(c), \\ e &= [1, \dots, 1]^T \in \mathbb{R}^r, & z_\varrho &= [1, 1/2, \dots, 1/\varrho]^T \in \mathbb{R}^\varrho \end{aligned}}. \quad (6)$$

$\mathcal{B}(\varrho)$  says that formula (4) has (at least) order  $\varrho$ .

$\mathcal{C}(\varrho)$  says that each of the interior formulas (3) has (at least) order  $\varrho$ .

By partial integration we obtain the relation

$$\int_0^1 x^k \int_0^x f(t) dt dx = \frac{1}{k+1} \int_0^1 (1-x^{k+1})f(x) dx, \quad k \in \mathbb{N}_0. \quad (7)$$

On choosing here the interior rules (3) for the interior integral at left and the exterior rule (4) else, we obtain

$$\sum_{i=1}^r \beta_i \gamma_i^k \sum_{j=1}^r a_{ij} f(\gamma_j) \simeq \frac{1}{k+1} \sum_{j=1}^r \beta_j (1-\gamma_j^{k+1}) f(\gamma_j). \quad (8)$$

Let  $j$  fixed and choose for  $f$  the polynomials  $\psi \in \Pi_{r-1}$  where  $\psi(\gamma_i) = \delta^i_j$  (Kronecker symbol), then

$$\sum_{i=1}^r \beta_i \gamma_i^k a_{ij} \simeq \frac{1}{k+1} \beta_j (1-\gamma_j^{k+1}), \quad j = 1 : r.$$

$\mathcal{D}(\varrho)$  says that this relation is exact for  $k = 0 : \varrho - 1$ .

Using (6), the conventions (5) are equivalent to

$$\boxed{\begin{aligned} \mathcal{A}(\varrho) &\iff \text{RKM has order } \varrho \\ \mathcal{B}(\varrho) &\iff b^T C^{k-1} e = \frac{1}{k}, & k &= 1 : \varrho \\ \mathcal{C}(\varrho) &\iff AC^{k-1} e = \frac{1}{k} C^k e, & k &= 1 : \varrho \\ \mathcal{D}(\varrho) &\iff b^T C^{k-1} A = \frac{1}{k} (b^T - b^T C^k), & k &= 1 : \varrho \\ \mathcal{E}(\varrho, \eta) &\iff b^T C^{k-1} A C^{\ell-1} e = \frac{1}{\ell(k+\ell)}, & k &= 1 : \varrho, \ell = 1 : \eta \end{aligned}}. \quad (9)$$

VANDERMONDE's matrix:

$$V_\varrho = [\gamma_i^{j-1}]_{i=1, j=1}^r = \begin{bmatrix} 1 & \gamma_1 & \gamma_1^2 & \dots & \gamma_1^{\varrho-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & \gamma_r & \gamma_r^2 & \dots & \gamma_r^{\varrho-1} \end{bmatrix} \in \mathbb{R}_\varrho^r$$

Matrices of HILBERT type:

$$H = \begin{bmatrix} 1 & \frac{1}{2} & \dots & \frac{1}{r} \\ \frac{1}{2} & \frac{1}{3} & \dots & \frac{1}{r+1} \\ \vdots & \vdots & & \vdots \\ \frac{1}{r} & \frac{1}{r+1} & \dots & \frac{1}{2r} \end{bmatrix} \in \mathbb{R}_r^r, \quad \tilde{H}_{\varrho, \eta} = \begin{bmatrix} \frac{1}{2} & \frac{1}{3} & \dots & \frac{1}{\eta+1} \\ \frac{1}{4} & \frac{1}{4} & \dots & \frac{1}{\eta+2} \\ \vdots & \vdots & & \vdots \\ \frac{1}{\varrho+1} & \frac{1}{\varrho+1} & \dots & \frac{1}{\varrho+\eta} \end{bmatrix} \in \mathbb{R}_\eta^{\varrho}$$

Using these notations (9) gets the form

$$\begin{array}{lcl}
 \mathcal{B}(\varrho) & \iff & V_\varrho^T b = z_\varrho \\
 \mathcal{C}(\varrho) & \iff & AV_\varrho = \text{diag}(c)V_\varrho \text{diag}(z_\varrho) =: W_\varrho \in \mathbb{R}^r \\
 \mathcal{D}(\varrho) & \iff & V_\varrho^T \text{diag}(b)A = (z_\varrho e^T - W_\varrho^T) \text{diag}(b) \\
 \mathcal{E}(\varrho, \eta) & \iff & V_\varrho^T \text{diag}(b)AV_\eta = \tilde{H}_{\varrho, \eta} z_\eta
 \end{array} \quad (10)$$

**Theorem 1** [Butcher1964] *Let a  $r$ -stage RKM be given with mutually different nodes  $\gamma_1, \dots, \gamma_r$ . Then*

$$\begin{array}{lcl}
 (1^\circ) & \mathcal{A}(\xi) & \implies \mathcal{B}(\xi) \\
 (2^\circ) & \mathcal{A}(\eta + \xi) & \implies \mathcal{E}(\eta, \xi) \\
 (3^\circ) & \mathcal{B}(\eta + \xi) \text{ und } \mathcal{C}(\xi) & \implies \mathcal{E}(\eta, \xi) \\
 (4^\circ) & \mathcal{B}(\eta + \xi) \text{ und } \mathcal{D}(\eta) & \implies \mathcal{E}(\eta, \xi) \\
 (5^\circ) & \mathcal{B}(\eta + r) \text{ und } \mathcal{E}(r, \xi) & \implies \mathcal{C}(\xi), \text{ wenn alle } \beta_i \neq 0 \\
 (6^\circ) & \mathcal{B}(\eta + r) \text{ und } \mathcal{E}(\eta, r) & \implies \mathcal{D}(\eta).
 \end{array}$$

*Proof.* Cf. [Crouzeix75], [Dekker].

(1°) Apply a RKM of order  $p$  to the differential equation  $x'(t) = f(t) \in \mathbb{R}$  then exact integration follows for  $f(t) = t^{k-1}$ ,  $k = 1 : \xi$  hence  $\mathcal{B}(\xi)$ .

*In detail.* For  $y'(t) = c(t) \in \mathbb{R}^m$  we have

$$d(t, x, \tau) = \frac{1}{\tau} \int_t^{t+\tau} c(t) dt - \sum_{j=1}^r \beta_j c(t_j), \quad t_j := t + \gamma_j \tau. \quad (11)$$

TAYLOR expansion at the point  $t$  yields

$$\begin{aligned}
 \int_t^{t+\tau} c(t) dt &= \sum_{k=0}^{p-1} \frac{\tau^{k+1}}{(k+1)!} c^{(k)}(t) + \mathcal{O}(\tau^{p+1}) \\
 \sum_{j=1}^r \beta_j c(t_j) &= \sum_{k=0}^{p-1} \sum_{j=1}^r \beta_j \frac{c^{(k)}(t)}{k!} (\gamma_j \tau)^k + \mathcal{O}(\tau^p) \\
 &= \sum_{k=0}^{p-1} \left( \sum_{j=1}^r \beta_j \gamma_j^k \right) \frac{\tau^k}{k!} c^{(k)}(t) + \mathcal{O}(\tau^p).
 \end{aligned}$$

Inserting into (11) yields

$$d(t, x, \tau) = \sum_{k=0}^{p-1} \left( \frac{1}{k+1} - \sum_{j=1}^r \beta_j \gamma_j^k \right) \frac{\tau^k}{k!} c^{(k)}(t) + \mathcal{O}(\tau^p)$$

By this way, we obtain as *necessary* condition for order  $p$  of a RKM that

$$\boxed{k = 1 : p : b^T C^{k-1} e = \frac{1}{k} \iff \mathcal{B}(p)}, \quad (12)$$

which shall always be fulfilled in the sequel.

(2°) A RKM of order  $p = \xi + \eta$  yields the exact solution for the system

$$\begin{aligned} x_1'(t) &= \ell t^{\ell-1}, & x_1(t_0) &= 0 \\ x_2'(t) &= (\ell + k)t^{k-1}x_1(t), & x_2(t_0) &= 0, \quad k = 1 : \eta, \ell = 1 : \xi \end{aligned}$$

which shows immediately the assertion.

(3°)

$$b^T C^{k-1} A C^{\ell-1} e \stackrel{\mathcal{C}(\xi)}{=} b^T C^{k-1} \frac{1}{\ell} C^\ell e = \frac{1}{\ell} b^T C^{k+\ell-1} e \stackrel{\mathcal{B}(\eta+\xi)}{=} \frac{1}{\ell(k+\ell)}, \quad k = 1 : \eta, \ell = 1 : \xi.$$

(4°)

$$\begin{aligned} b^T C^{k-1} A C^{\ell-1} e &\stackrel{\mathcal{D}(\eta)}{=} \frac{1}{k} (b^T - b^T C^k) C^{\ell-1} e = \frac{1}{k} (b^T C^{\ell-1} e - b^T C^{k+\ell-1} e) \\ &\stackrel{\mathcal{B}(\eta+\xi)}{=} \frac{1}{k} \left( \frac{1}{\ell} - \frac{1}{k+\ell} \right) = \frac{1}{\ell(k+\ell)}, \quad k = 1 : \eta, \ell = 1 : \xi. \end{aligned}$$

(5°) From  $\mathcal{B}(\xi + r)$  and  $\mathcal{E}(r, \xi)$  there follows

$$\begin{aligned} 0 &= \frac{1}{\ell(k+\ell)} - \frac{1}{\ell(k+\ell)} = b^T C^{k-1} A C^{\ell-1} e - \frac{1}{\ell} C^{k+\ell-1} e \\ &= b^T C^{k-1} \left( A C^{\ell-1} e - \frac{1}{\ell} C^\ell e \right), \quad k = 1 : r, \ell = 1 : \xi. \end{aligned}$$

These are  $r$  homogeneous linear equations with regular matrix of coefficients, because all  $\gamma_i$  are mutually distinct and all weights  $\beta_i$  are nonzero by assumption. Therefore all bracketed terms (being the variables) must disappear. This yields assertion  $\mathcal{C}(\xi)$ .

(6°) By  $\mathcal{E}(\eta, r)$  we obtain

$$b^T C^{k-1} A C^{\ell-1} e = e^T C^{\ell-1} (A^T C^{k-1} b) = \frac{1}{\ell(k+\ell)}, \quad k = 1 : \eta, \ell = 1 : r$$

and form  $\mathcal{B}(\eta + r)$  by transposition

$$\frac{1}{k} (e^T C^{\ell-1} b - e^T C^{k+\ell-1} b) = e^T C^{\ell-1} \frac{1}{k} (b - C^k b) = \frac{1}{k} \left( \frac{1}{\ell} - \frac{1}{k+\ell} \right), \quad k = 1 : \eta, \ell = 1 : r$$

The difference yields

$$e^T C^{\ell-1} \left( A^T C^{k-1} b - \frac{1}{k} (b - C^k b) \right) = 0, \quad k = 1 : \eta, \ell = 1 : r$$

These are again  $r$  homogeneous linear equations with regular matrix of coefficients for the bracketed terms because all  $\gamma_i$  shall be different which yields the assertion  $\mathcal{D}(\eta)$ .  $\square$

**Theorem 2** [Butcher1964] *Let a  $r$ -stage RKM be given where all nodes  $\gamma_1, \dots, \gamma_r$  are mutually distinct. Then*

(1°)  $\mathcal{A}(\varrho + r) \implies \mathcal{B}(\varrho + r)$  and  $\mathcal{D}(r)$ ,

(2°)  $\mathcal{A}(\varrho + r) \implies \mathcal{C}(r)$ , if all weights  $\beta_i \neq 0$ ,

(3°)  $\mathcal{B}(\varrho + r) \wedge \mathcal{C}(r) \implies \mathcal{D}(\varrho)$ ,

(4°)  $\mathcal{B}(\varrho + r) \wedge \mathcal{D}(r) \implies \mathcal{C}(\varrho)$ , if all weights  $\beta_i \neq 0$ .

*Proof.* Cf. [Crouzeix75], [Dekker].

(1°) follows from Theorem 1, (1°), (2°), (6°).

(2°) follows from Theorem 1, (1°), (2°), (5°).

(3°) follows from Theorem 1, (3°), (6°).

(4°) follows from Theorem 1, (4°), (5°).

□

**Theorem 3** [Butcher1964] *Let a  $r$ -stage RKM be given where all nodes  $\gamma_1, \dots, \gamma_r$  are mutually distinct and all weights  $\beta_1, \dots, \beta_r$  are different from zero. Then*

$$\mathcal{B}(\varrho) \text{ and } \mathcal{C}(\xi) \text{ and } \mathcal{D}(\eta) \implies \mathcal{A}(p), \quad p = \min\{\varrho, \xi + \eta + 1, 2\xi + 2\}.$$

[Crouzeix75], see also [Crouzeix80], has proved this result by using algebraic/analytic auxiliaries and not the difficult BUTCHER technique. Since the indicated original reference is difficult to get, the proof is given here in full length. To this end there at first necessary and sufficient conditions for order  $p$  of a  $r$ -stage RKM in linear systems (2) necessary.

We use the notations of the book and of (5). By § 2.4(d)(4°), let  $Z(t)$  be the solution of the implicit system of interior equations,

$$Z(t) = e \times x(t) + \tau(A \times I)F(t, Z(t)), \quad (13)$$

( $\tau > 0$  step length), then

$$d(t, x, \tau) = \frac{x(t + \tau) - x(t)}{\tau} - (b \times I)^T F(t, Z(t)) \quad (14)$$

is the discretization error and the RKM has order  $p$  if  $d(t, x, \tau) = \mathcal{O}(\tau^p)$ .

□

**Assumption 1** *Let  $p \in \mathbb{N}$  fixed.*

(1°) *Suppose  $\mathcal{B}(p)$ ,*

$$b^T C^{k-1} e = \frac{1}{k}, \quad k = 1 : \varrho.$$

(2°) *Suppose*

$$\boxed{\begin{aligned} &\forall k \in \mathbb{N} \quad \forall s, \lambda_i \in \mathbb{N}_0 : k + \lambda_0 + \lambda_1 + \dots + \lambda_s \leq p - 1 - s \implies \\ &b^T C^{\lambda_0} A C^{\lambda_1} \dots A C^{\lambda_s} \left( \frac{1}{k} C^k - A C^{k-1} \right) e = 0 \end{aligned}} \quad (15)$$

**Theorem 4** *A  $r$ -stage RKM has order  $p$  for every linear system (2) if and only if Assumption 1 is fulfilled.*

*Proof.* (1°) For  $B(t) = 0$  we have

$$d(t, x, \tau) = \frac{1}{\tau} \int_t^{t+\tau} c(t) dt - \sum_{j=1}^r \beta_j c(t_j), \quad t_j := t + \gamma_j \tau. \quad (16)$$

TAYLOR expansion at the point  $t$  yields

$$\begin{aligned} \int_t^{t+\tau} c(t) dt &= \sum_{k=0}^{p-1} \frac{\tau^{k+1}}{(k+1)!} c^{(k)}(t) + \mathcal{O}(\tau^{p+1}) \\ \sum_{j=1}^r \beta_j c(t_j) &= \sum_{k=0}^{p-1} \sum_{j=1}^r \beta_j \frac{c^{(k)}(t)}{k!} (\gamma_j \tau)^k + \mathcal{O}(\tau^p) \\ &= \sum_{k=0}^{p-1} \left( \sum_{j=1}^r \beta_j \gamma_j^k \right) \frac{\tau^k}{k!} c^{(k)}(t) + \mathcal{O}(\tau^p). \end{aligned}$$

Inserting in (16) yields

$$d(t, x, \tau) = \sum_{k=0}^{p-1} \left( \frac{1}{k+1} - \sum_{j=1}^r \beta_j \gamma_j^k \right) \frac{\tau^k}{k!} c^{(k)}(t) + \mathcal{O}(\tau^p)$$

By this way, we obtain the following *necessary* condition for a RKM to have order  $p$ :

$$\boxed{k = 0 : (p-1) : b^T C^k e = \frac{1}{k+1} \iff \mathcal{B}(p)}, \quad (17)$$

which shall be always fulfilled in the sequel.

(2°)  $B(t) \neq 0$ . Let

$$\begin{aligned} \varepsilon_i &= y(t_i) - y(t) - \tau \sum_{j=1}^r a_{ij} y'(t_j), \quad t_i = t + \gamma_i \tau, \\ \eta &= \frac{y(t+\tau) - y(t)}{\tau} - \sum_{j=1}^r \beta_j y'(t_j). \end{aligned} \quad (18)$$

Inserting in (13) and (14) yields

$$\begin{aligned} y(t_i) - z_i &= \varepsilon_i + \tau \sum_{j=1}^r a_{ij} B(t_j) [y(t_j) - z_j] \\ d(t, x, \tau) &= \eta + \sum_{j=1}^r \beta_j B(t_j) [y(t_j) - z_j]. \end{aligned}$$

Using the notations

$$\varepsilon = [\varepsilon_1, \dots, \varepsilon_r]^T, \quad \mathbf{B} = \text{diag}(B(t_1), \dots, B(t_r))$$

we obtain

$$d(t, x, \tau) = b^T \mathbf{B} (I - \tau \mathbf{A} \mathbf{B})^{-1} \varepsilon + \eta.$$

TAYLOR expansion at the point  $t$  yields

$$\varepsilon_i = \sum_{k=1}^{p-1} \frac{\tau^k}{(k-1)!} \left( \frac{\gamma_i^k}{k} - \sum_{j=1}^r a_{ij} \gamma_j^{k-1} \right) y^{(k)}(t) + \mathcal{O}(\tau^p)$$

together

$$\varepsilon = \sum_{k=1}^{p-1} \frac{\tau^k}{(k-1)!} y^{(k)}(t) \left( \frac{1}{k} C^k - A C^{k-1} \right) e + \mathcal{O}(\tau^p) \quad (19)$$

On the other side, gilt  $\eta = \mathcal{O}(\tau^p)$  does hold by (18), whereby we obtain altogether

$$d(t, x, \tau) = \sum_{k=1}^{p-1} \frac{\tau^k}{(k-1)!} y^{(k)}(t) b^T \mathbf{B} (I - \tau \mathbf{A} \mathbf{B})^{-1} \left[ \frac{1}{k} C^k - A C^{k-1} \right] e + \mathcal{O}(\tau^p)$$

Setting here successively  $c(t) = kt^{k-1}y_0 - t^k B(t)y_0$  for  $k = 1 : (p-1)$ , then the linear system (2) has the solution  $y(t) = t^k y_0$  and for a RKM of order  $p$  there follows the condition

$$\boxed{\forall k = 1 : (p-1) : b^T \mathbf{B} (I - \tau \mathbf{A} \mathbf{B})^{-1} \left( \frac{1}{k} - A C^{k-1} \right) e = \mathcal{O}(\tau^{p-k})}. \quad (20)$$

By this way, a RKM has order  $p$  for a linear system (2) if and only if the conditions  $\mathcal{B}(p)$  and (20) are fulfilled.

(3°) For sufficiently small  $\tau > 0$  we have

$$(I - \tau \mathbf{A} \mathbf{B})^{-1} = I + \tau \mathbf{A} \mathbf{B} + \dots + \tau^\ell (\mathbf{A} \mathbf{B})^\ell + \mathcal{O}(\tau^{\ell+1}),$$

therefore (20) is equivalent to

$$\forall k = 1 : (p-1) : \sum_{\ell=0}^{p-k-1} \tau^\ell b^T \mathbf{B} (\mathbf{A} \mathbf{B})^\ell \left( \frac{1}{k} C^k - A C^{k-1} \right) e = \mathcal{O}(\tau^{p-k}), \quad (21)$$

on the other side

$$\mathbf{B} = \sum_{i=0}^s \frac{\tau^i}{i!} B^{(i)}(t) C^i + \mathcal{O}(\tau^{s+1}).$$

Therefore (21) is equivalent to the condition:

For  $k = 1 : (p-1)$

$$\sum_{s=0}^{p-k-1} \left[ \tau^s \sum_{\ell+i_0+\dots+i_\ell=s, \ell \geq 0, i_j \geq 0} \frac{B^{(i_0)}(t) \cdots B^{(i_\ell)}(t)}{i_0! \cdots i_\ell!} b^T C^{i_0} A C^{i_1} \cdots A C^{i_\ell} \left( \frac{1}{k} C^k - A C^{k-1} \right) e \right] = \mathcal{O}(\tau^{p-k})$$

This result however says: For all  $k = 1 : (p-1)$  and all  $s = 1 : (p-k-1)$  we have

$$\sum_{\ell+i_0+\dots+i_\ell=s} \frac{B^{(i_0)}(t) \cdots B^{(i_\ell)}(t)}{i_0! \cdots i_\ell!} b^T C^{i_0} A C^{i_1} \cdots A C^{i_\ell} \left( \frac{1}{k} C^k - A C^{k-1} \right) e = 0. \quad (22)$$

These relations must hold for every  $p$ -times differentiable matrix  $B(t)$ , therefore one can choose arbitrary functions for the derivatives  $B^{(i)}(t)$ ,  $i = 0 : (p-1)$ , e.g.  $B^{(i)}(t) = i! B_i$ .

Result: in order that (22) holds for every regular funktion  $B(t)$ , it is necessary and sufficient that:

For all  $B_0, B_1, \dots, B_{p-1} \in \mathbb{R}^m_m$  and for all  $k, s \in \mathbb{N}_0$  mit  $k + s \leq p - 1$  :

$$\sum_{\ell+i_0+\dots+i_\ell=s} B_{i_0} B_{i_1} \cdots B_{i_\ell} b^T C^{i_0} A C^{i_1} \cdots A C^{i_\ell} \left( \frac{1}{k} C^k - A C^{k-1} \right) e = 0. \quad (23)$$

Every real polynomial of several variables of degree  $\leq 2m-1$  disappearin identically on the ring of  $(m, m)$ -matrizes, is identically zero. (Theorem of AMITSUR-LEVITZKI). Thus, for  $2m \geq p$ , (23) is equivalent to:

For all  $k \geq 1$ , for all  $\ell \geq 0$ , for all  $i_0, i_1, \dots, i_\ell \geq 0$  such that  $k + \ell + i_0 + i_1 + \dots + i_\ell \leq p - 1$ , the following relation does hold

$$b^T C^{i_0} A C^{i_1} \dots A C^{i_\ell} \left( \frac{1}{k} C^k - A C^{k-1} \right) e = 0. \quad (24)$$

Accordingly, a RKM has order  $p$  for arbitrary linear systems (2) if and only if (17) and (24) are fulfilled.  $\square$

*Remark.* In order to show that the conditions of Theorem 4 are necessary, it has been supposed that  $m \geq 2p$  does hold for the dimension of the linear system (2). This condition is certainly not optimal. For instance, the conditions (15) are no longer all necessary in case  $m = 1$  and  $p \geq 4$ .

Consider a linear system (2) with constant matrix  $B$ ,

$$x'(t) = Bx(t) + c(t) \in \mathbb{R}^m \quad (25)$$

Then the following result does hold:

**Theorem 5** *A  $r$ -stage RKM has order  $p$  for all sufficient smooth systems (25) if and only if*

$$b^T A^{k-\ell} C^\ell e = \prod_{i=\ell}^k \frac{1}{i+1}, \quad k = 0 : (p-1), \quad \ell = 0 : k. \quad (26)$$

*Proof.* The proof of Theorem 4 remains the same up to formula (21), but now  $\mathbf{B} = BI$  (in fact  $B \times I$ , KRONECKER product). Then, by (21), for  $k = 1 : (p-1)$

$$\sum_{\ell=0}^{p-k-1} B^\ell \tau^\ell b^T A^\ell \left( \frac{1}{k} C^k - A C^{k-1} \right) e = \mathcal{O}(\tau^{p-k}). \quad (27)$$

This condition is equivalent to:  $\forall k \geq 1 \quad \forall \ell \geq 0 : k + \ell \leq p - 1 \implies$

$$b^T A^\ell \left( \frac{1}{k} C^k - A C^{k-1} \right) e = 0. \quad (28)$$

Therefore a RKM has order  $p$  for every system (25) if and only if (17) and (28) are fulfilled. These two conditions follow apparently from (26). Conversely, it can be shown easily by recurrence that (17) and (28) determine uniquely the values  $b^T A^{k-\ell} C^\ell e$  for all  $0 \leq \ell \leq k \leq p - 1$ . Therefore (26) is in the mentioned case equivalent to (17) and (28).

Condition (26) is also fulfilled in the case  $m = 1$ .

We now return to the general nonlinear differential system (1), namely to Theorem 3.

**Theorem** Let a  $r$ -stage RKM be given where all nodes  $\gamma_1, \dots, \gamma_r$  are mutually distinct and all weights  $\beta_1, \dots, \beta_r$  are non-zero. Then

$$\mathcal{B}(\varrho) \text{ and } \mathcal{C}(\xi) \text{ and } \mathcal{D}(\eta) \implies \mathcal{A}(p), \quad p = \min\{\varrho, \xi + \eta + 1, 2\xi + 2\}.$$

*Proof.* Let  $y$  be a solution of  $y'(t) = f(t, y(t))$  and let

$$B(t) = \text{grad}_y f(t, y(t)), \quad c(t) = f(t, y(t)) - B(t)y(t),$$



then  $y$  is also solutin of

$$y'(t) = B(t)y(t) + c(t).$$

We consider the following quantities:

$$\begin{aligned} z_i &:= y(t) + \tau \sum_{j=1}^r a_{ij} f(t_j, z_j), \quad t_j = t + \gamma_j \tau \\ E &:= \frac{y(t + \tau) - y(t)}{\tau} - \sum_{j=1}^r \beta_j f(t_j, z_j) \end{aligned} \quad (29)$$

$$\begin{aligned} \zeta_i &:= y(t) + \tau \sum_{j=1}^r a_{ij} [B(t_j)\zeta_j + c(t_j)] \\ \varepsilon &:= \frac{y(t + \tau) - y(t)}{\tau} - \sum_{j=1}^r \beta_j [B(t_j)\zeta_j + c(t_j)]. \end{aligned} \quad (30)$$

Furthermore, because  $\mathcal{C}(\xi)$ ,

$$d := AC^\xi e - \frac{1}{\xi + 1} C^{\xi+1} e \neq 0$$

then, by (18) and 19),

$$y(t_i) = y(t) + \tau \sum_{j=1}^r a_{ij} f(t_j, y(t_j)) - \frac{\tau^{\xi+1}}{\xi!} d_i y^{(\xi+1)}(t) + \mathcal{O}(\tau^{\xi+2})$$

By this way, we obtain

$$z_i - y(t_i) = \tau \sum_{j=1}^r a_{ij} [f(t_j, z_j) - f(t_j, y(t_j))] + \frac{\tau^{\xi+1}}{\xi!} d_i y^{(\xi+1)}(t) + \mathcal{O}(\tau^{\xi+2}). \quad (31)$$

The function  $f$  shall be sufficiently smooth therefore it locally LIPSCHITZ-continuous, and we obtain

$$\sum_{i=1}^r |z_i - y(t_i)| \leq rL\tau \max_{i,j=1}^r |a_{ij}| \sum_{i=1}^r |z_i - y(t_i)| + \mathcal{O}(\tau^{\xi+1}).$$

Accordingly,

$$\sum_{i=1}^r |z_i - y(t_i)| = \mathcal{O}(\tau^{\xi+1}).$$

and, after inserting in (31),

$$z_i - y(t_i) = \frac{\tau^{\xi+1}}{\xi!} d_i y^{(\xi+1)}(t) + \mathcal{O}(\tau^{\xi+2}). \quad (32)$$

On the other side

$$f(t_i, z_i) = f(t_i, y(t_i)) + B(t_i)[z_i - y(t_i)] + \frac{\partial^2 f}{\partial y^2}(t_i, y(t_i))[z_i - y(t_i)]^2 + \mathcal{O}(\tau^{3\xi+3})$$

and

$$B(t_i)\zeta_i + c(t_i) = f(t_i, y(t_i)) + B(t_i)[\zeta_i - y(t_i)]$$

We write briefly

$$K = \frac{\partial^2 f}{\partial y^2}(t, y(t))[y^{(\xi+1)}(t)]^2$$

and obtain by using (32)

$$f(t_i, z_i) - [B(t_i)\zeta_i + c(t_i)] = B(t_i)[z_i - \zeta_i] + d_i^2 \frac{\tau^{2\xi+2}}{(s!)^2} K + \mathcal{O}(\tau^{2\xi+3}) \quad (33)$$

which yields, by inserting into (29) and (30),

$$z_i - \zeta_i = \tau \sum_{j=1}^r a_{ij} B(t_j)(z_j - \zeta_j) + \mathcal{O}(\tau^{2\xi+3})$$

therefore

$$z_i - \zeta_i = \mathcal{O}(\tau^{2\xi+3}).$$

Inserting in (33) yields

$$f(t_i, z_i) - [B(t_i)\zeta_i + c(t_i)] = d_i^2 \frac{\tau^{2\xi+2}}{(\xi!)^2} K + \mathcal{O}(\tau^{2\xi+3}).$$

However, by (29) and (30),

$$E = \varepsilon - \sum_{i=1}^r \beta_i [f(t_i, z_i) - B(t_i)\zeta_i - c(t_i)].$$

Therefore

$$E = \varepsilon - \left[ \sum_{i=1}^r \beta_i d_i^2 \right] \frac{\tau^{2\xi+2}}{(\xi!)^2} K + \mathcal{O}(\tau^{2s+3}). \quad (34)$$

Thus it is to be shown that

$$\varepsilon = \mathcal{O}(\tau^{x+\eta+1}). \quad (35)$$

Or, by Theorem 4 it is to be shown that

$$\mathcal{B}(\varrho) \wedge \mathcal{C}(\xi) \wedge \mathcal{D}(\eta) \implies \text{Vor. 3 f\"ur } p = \xi + \eta + 1.$$

Remember:

$$\begin{aligned} \mathcal{B}(\varrho) &\iff b^T C^{k-1} e = \frac{1}{k}, & k = 1 : \varrho \\ \mathcal{C}(\xi) &\iff AC^{k-1} e = \frac{1}{k} C^k e, & k = 1 : \xi \\ \mathcal{D}(\eta) &\iff b^T C^{k-1} A = \frac{1}{k} (b^T - b^T C^k), & k = 1 : \eta \end{aligned} \quad (36)$$

By assumption  $\mathcal{B}(\xi + \eta + 1)$  it is to be shown:

$$\boxed{\begin{aligned} \forall k \in \mathbb{N} \quad \forall s, \lambda_i \in \mathbb{N}_0 : k + \lambda_0 + \lambda_1 + \dots + \lambda_s \leq \xi + \eta + 1 - 1 - s \implies \\ b^T C^{\lambda_0} A C^{\lambda_1} \dots A C^{\lambda_s} \left( \frac{1}{k} C^k - A C^{k-1} \right) e = 0 \end{aligned}} \quad (37)$$

Suppose now  $\mathcal{B}(\xi + \eta + 1)$  and  $\mathcal{C}(\xi)$  then it is to show that

$$\boxed{\begin{aligned} \forall k \in \mathbb{N} \quad \forall s, \lambda_i \in \mathbb{N}_0 : k + \lambda_0 + \lambda_1 + \dots + \lambda_s \leq \eta - s \implies \\ b^T C^{\lambda_0} A C^{\lambda_1} \dots A C^{\lambda_s} \left( \frac{1}{\xi + k} C^{\xi+k} - A C^{\xi+k-1} \right) e = 0 \end{aligned}} \quad (38)$$

(1°)  $s = 0$  Then it is to show that

$$b^T C^\lambda \left( \frac{1}{\xi + k} C^{\xi+k} - AC^{\xi+k-1} \right) e = 0, \quad 0 \leq \lambda + k \leq \eta \quad (39)$$

From  $\mathcal{B}(\xi + \eta + 1)$  we obtain

$$\frac{1}{\xi + k} b^T C^{\lambda+\xi+k} e = \frac{1}{(\xi + k)(\lambda + \xi + k + 1)}$$

From  $\mathcal{B}(\xi + \eta + 1)$  and  $\mathcal{D}(\eta)$  we obtain

$$b^T C^\lambda AC^{\xi+k-1} e = \frac{1}{\lambda + 1} (b^T - b^T C^{\lambda+1}) C^{\xi+k-1} e = \frac{1}{\lambda + 1} \left( \frac{1}{\xi + k} - \frac{1}{\lambda + \xi + k + 1} \right)$$

This relation yields (39).

(2°) Let the assertion (38) be true for  $s$  fixed.

(3°) It is to show that we obtain by (2°)

$$\begin{aligned} & \forall k \in \mathbb{N} \quad \forall \lambda, \lambda_i \in \mathbb{N}_0 : k + \lambda + \lambda_0 + \lambda_1 + \dots + \lambda_s \leq \eta - (s + 1) \implies \\ & b^T C^\lambda AC^{\lambda_0} AC^{\lambda_1} \dots AC^{\lambda_s} \left( \frac{1}{\xi + k} C^{\xi+k} - AC^{\xi+k-1} \right) e = 0 \end{aligned} \quad (40)$$

By  $\mathcal{D}(\eta)$  we but have

$$b^T C^\lambda A = \frac{1}{\lambda + 1} (b^T - b^T C^{\lambda+1})$$

Inserting yields

$$\begin{aligned} & b^T C^\lambda AC^{\lambda_0} AC^{\lambda_1} \dots AC^{\lambda_s} \left( \frac{1}{\xi + k} C^{\xi+k} - AC^{\xi+k-1} \right) e \\ &= \frac{1}{\lambda + 1} \left[ b^T C^{\lambda_0} AC^{\lambda_1} \dots AC^{\lambda_s} \left( \frac{1}{\xi + k} C^{\xi+k} - AC^{\xi+k-1} \right) e \right] \\ & \quad - \frac{1}{\lambda + 1} \left[ b^T C^{\lambda+\lambda_0+1} AC^{\lambda_1} \dots AC^{\lambda_s} \left( \frac{1}{\xi + k} C^{\xi+k} - AC^{\xi+k-1} \right) e \right] \end{aligned}$$

By induction hypothesis, both factors are zero.  $\square$

**Lemma 1** *The following two assumptions are equivalent for fixed  $p \in \mathbb{N}$ :*

**Assumption 2** *Let  $p \in \mathbb{N}$  fixed. Suppose  $\mathcal{B}(p)$  and*

$$\boxed{\begin{aligned} & \forall k \in \mathbb{N} \quad \forall s, \lambda_i \in \mathbb{N}_0 : k + \lambda_0 + \lambda_1 + \dots + \lambda_s \leq p - 1 - s \implies \\ & b^T C^{\lambda_0} AC^{\lambda_1} \dots AC^{\lambda_s} \left( \frac{1}{k} C^k - AC^{k-1} \right) e = 0 \end{aligned}} \quad (41)$$

and

**Assumption 3** Let  $p \in \mathbb{N}$  fixed. Let

$$\boxed{\begin{aligned} &\forall s \in \mathbb{N} \quad \forall \lambda_k \in \mathbb{N}_0 : \sum_{k=1}^s \lambda_k \leq p - s \implies \\ &b^T C^{\lambda_1} A C^{\lambda_2} \dots A C^{\lambda_s} e = \prod_{i=1}^s \left[ (s - i + 1) + \sum_{k=i}^s \lambda_k \right]^{-1} \end{aligned}} \quad (42)$$

In particular

$$\begin{aligned} s = 1 : & \quad b^T C^{\lambda_1} A C^{\lambda_2} \dots A C^{\lambda_s} = b^T C^{\lambda_1} e \\ s = 2 : & \quad b^T C^{\lambda_1} A C^{\lambda_2} \dots A C^{\lambda_s} = b^T C^{\lambda_1} A C^{\lambda_2} e. \end{aligned}$$

Assumption 2 is apparently more simple but Assumption 3 is somewhat more advantageous for the calculation of concrete conditions.

*Proof.* Assumption 2 is trivially equivalent to  $\mathcal{B}(p)$ ; Assumption 3 is equivalent to  $\mathcal{B}(p)$  for  $s = 1$ . It follows by induction that  $\mathcal{B}(p)$  and Assumption 2 determine uniquely the value

$$b^T C^{\lambda_1} A C^{\lambda_2} \dots A C^{\lambda_s} e$$

for all  $s \in \mathbb{N}$  and all  $\lambda_1, \lambda_2, \dots, \lambda_s \in \mathbb{N}_0$  such that  $\lambda_1 + \dots + \lambda_s \leq p - s$ . Accordingly, for equivalence it is only to show that Assumption 3 implies Assumption 2 which is left to the reader.  $\square$

**Lemma 2** There exists exactly one  $r$ -stage RKM of order  $2r$ . It is determined by  $\mathcal{B}(2r)$  and  $\mathcal{C}(r)$ .

*Proof.* There exists exactly one integration rule of order  $2r$  for the exterior equation

$$\int_0^1 f(t) dt \sim \sum_{i=1}^r \beta_i f(\gamma_i)$$

namely the GAUSS-LEGENDRE formula with  $r$  nodes in interval  $[0, 1]$ . Their weights  $\beta_i$ ,  $i = 1 : r$  are all positive. Then, because of Theorem 2(3°) we obtain  $\mathcal{D}(r)$  and thus by Theorem 3 for the order  $p$

$$p = \min\{2r, 2r + 1, 2r + 2\} = 2r.$$

Moreover, it follows from (10) that the matrix  $A = WV^{-1}$  in  $\mathcal{C}(r)$  is determined uniquely.  $\square$

Literatur: [Hairer], [Shampine97] und

Dekker, K., Verwer, J.G.: Stability of Runge-Kutta Methods for stiff nonlinear differential equations. North Holland, Amsterdam (1984)

Crouzeix, M.: Sur l'approximation des equations differentielles operationelles lineaires par des methods de Runge-Kutta. Thesis. Universite de Paris (1975).

Crouzeix, M., Raviart, P.-A.: Approximation des Problemes d'Evolution. Unver"offentliches Vorlesungsskript. Universite de Rennes (1980).