Differential-algebraic equations. Control and Numerics II

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Outline

Differential-algebraic equations (DAEs)

We have consider general nonsquare DAE

$$0 = \mathcal{F}(t, x, \dot{x}),\ x(t_0) = x_0,$$

with $F \in C^0(\mathbb{R} \times \mathbb{D}_x \times \mathbb{D}_{\dot{x}}, \mathbb{R}^\ell)$,
In the linear case (linearization along non-stationary solutions) we get

$$E(t)\dot{x} = A(t)x + f(t),\ x(t_0) = x_0,$$

or

$$E\dot{x} = Ax + f(t),\ x(t_0) = x_0.$$

Existence, uniqueness, consistency

Theorem (Kunkel/M. 1994)

Let the s-index μ be well–defined for $(E(t), A(t))$ and let $f \in C^{\mu}(\mathbb{I}, \mathbb{C}^{l})$. Then the system is equivalent to a remodeled DAE in normal form

$$\begin{array}{rcll} \dot{x}_1(t) & = & A_{13}(t)x_3(t) + f_1(t), & d_\mu \text{ equations}, \\ 0 & = & x_2(t) + f_2(t), & a_\mu \text{ equations}, \\ 0 & = & f_3(t), & v_\mu \text{ equations}, \end{array}$$

where the inhomogeneity is determined by $f^{(0)}, \ldots, f^{(\mu)}$.

- ▷ *The problem is solvable if and only if $f_3(t) \equiv 0$.*
- ▷ *An initial condition is consistent if and only if in addition $x_2(t_0) = -f_2(t_0)$ holds.*
- ▷ *The problem is uniquely solvable if again in addition we have $u_\mu = n - d_\mu - a_\mu = 0$.*

Evaluation of the algebraic approach

- The algebraic approach is essential for the theoretical understanding of DAEs.
- It can be used to study controllable, observable, autonomous behavior in the sense of Willems, see Ilchmann/M. 2005.
- The approach allows to do bifurcation analysis, the points where ranks change are a superset of the set of *critical points*.
- But, it cannot be used for the nonlinear case, for numerical methods or the design of controllers, since one would need derivatives of computed transformation matrices.

Outline

For numerical methods and for the design of controllers, we use derivative arrays (Campbell 1989). We assume that derivatives of original functions are available or can be obtained via computer algebra or automatic differentiation.

Linear case: We put $E(t)\dot{x} = A(t)x + f(t)$ and its derivatives up to order μ into a large DAE

$$M_k(t)\dot{z}_k = N_k(t)z_k + g_k(t), \quad k \in \mathbb{N}_0$$

for $z_k = [x^T, \dot{x}^T, \ldots, {x^{(k)}}^T]$.

$$M_2 = \begin{bmatrix} E & 0 & 0 \\ A - \dot{E} & E & 0 \\ \dot{A} - 2\ddot{E} & A - \dot{E} & E \end{bmatrix}, \; N_2 = \begin{bmatrix} A & 0 & 0 \\ \dot{A} & 0 & 0 \\ \ddot{A} & 0 & 0 \end{bmatrix}, \; z_2 = \begin{bmatrix} x \\ \dot{x} \\ \ddot{x} \end{bmatrix}.$$

Theorem (Kunkel/M. 1996)

Under some constant rank assumptions, for every linear DAE there exist integers μ, a, d and v such that:

1. $\operatorname{corank} M_{\mu+1}(t) - \operatorname{corank} M_{\mu}(t) = v$.
2. $\operatorname{rank} M_{\mu}(t) = (\mu+1)m - a - v$ *on* $\mathbb{I}$, *and there exists a smooth matrix function* $Z_{2,3}$ *(left nullspace of* M_μ*) with* $Z_{2,3}^T M_\mu(t) = 0$.
3. *The projection* $Z_{2,3}$ *can be partitioned into two parts:* Z_2 *(left nullspace of* (M_μ, N_μ)*) so that the first block column* $\hat{A}_2$ *of* $Z_2^* N_\mu(t)$ *has full rank* a *and* $Z_3^* N_\mu(t) = 0$. *Let* T_2 *be a smooth matrix function such that* $\hat{A}_2 T_2 = 0$, *(right nullspace of* $\hat{A}_2$*).*
4. $\operatorname{rank} E(t) T_2 = d = \ell - a - v$ *and there exists a smooth matrix function* Z_1 *of size* (n, d) *with* $\operatorname{rank} \hat{E}_1 = d$, *where* $\hat{E}_1 = Z_1^T E$.

- $Z_{2,3}^T$ operates on the derivative array

$$M_\mu(t)\dot{z}_\mu = N_\mu(t)z_\mu + g_\mu(t),$$

and picks out the algebraic and the redundant part.

- It extracts all constraint equations including redundancies (Z_3^T) and all explicit and implicit (hidden) constraints (Z_2^T.
- Z_1^T operates on the original system

$$E(t)\dot{x} = A(t)x + f(t),$$

and picks out the dynamic part.

Reduced problem, remodeled DAE

We obtain a numerically computable **strangeness-free condensed form**

$$\begin{array}{rcll} \hat{E}_1(t)\dot{x} & = & \hat{A}_1(t)x + \hat{f}_1(t), & d_\mu \text{ equations} \\ 0 & = & \hat{A}_2(t)x + \hat{f}_2(t), & a_\mu \text{ equations} \\ 0 & = & \hat{f}_3(t), & v_\mu \text{ equations} \end{array}$$

where $\hat{A}_1 = Z_1^T A$, $\hat{f}_1 = Z_1^T f$, and $\hat{f}_2 = Z_2^T g_\mu$, $\hat{f}_3 = Z_3^T g_\mu$.
The partitioning is the same as in the canonical form

$$\begin{array}{rcll} \dot{x}_1(t) & = & A_{13}(t)x_3(t) + f_1(t), & d \text{ equations} \\ 0 & = & x_2(t) + f_2(t), & a \text{ equations} \\ 0 & = & f_3(t), & v \text{ equations.} \end{array}$$

Circuit model as linear DAE with constant coefficients
$E\dot{x} = Ax + f$.

$$\begin{bmatrix} 0 & C & C \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1/R & 1/R & 0 \\ 1 & 0 & -1 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} - \begin{bmatrix} 0 \\ U \\ 0 \end{bmatrix}$$

Derivative array

$$\left[\begin{array}{ccc|ccc} 0 & C & C & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \hline R^{-1} & -R^{-1} & 0 & 0 & C & C \\ 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{array}\right] \left[\begin{array}{c} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \hline \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \end{array}\right] = \left[\begin{array}{ccc|ccc} -R^{-1} & R^{-1} & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] \left[\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ \hline \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{array}\right] - \left[\begin{array}{c} 0 \\ U \\ 0 \\ \hline 0 \\ 0 \\ 0 \end{array}\right].$$

$$Z_{2,3}^T = \left[\begin{array}{ccc|ccc} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{array}\right], \; Z_{2,3}^T N_1 I_3 = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 1 \end{bmatrix}$$

has full row rank, hence $Z_{2,3}^T = Z_2^T$ and Z_3 is void.

$$\hat{A}_2 = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 1 \end{bmatrix}, \; \hat{f}_2 = \begin{bmatrix} -U \\ 0 \end{bmatrix}, \; T_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}.$$

$$ET_2 = \begin{bmatrix} C \\ 0 \\ 0 \end{bmatrix}, \; Z_1^T = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}$$

$$\hat{E}_1 = \begin{bmatrix} 0 & C & C \end{bmatrix}, \; \hat{A}_1 = \begin{bmatrix} -R^{-1} & R^{-1} & 0 \end{bmatrix}, \; \hat{f}_1 = 0.$$

$$\begin{aligned} C(\dot{x}_3 - \dot{x}_2) + (x_1 - x_2)/R &= 0, \\ x_1 - x_3 - U &= 0, \\ x_3 &= 0. \end{aligned}$$

DAE

$$\begin{bmatrix} 0 & C & C \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1/R & 1/R & 0 \\ 1 & 0 & -1 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} - \begin{bmatrix} 0 \\ U \\ 0 \end{bmatrix}$$

Remodeled strangeness-free DAE

$$\left[\begin{array}{c|cc} 0 & C & C \\ \hline 0 & 0 & 0 \\ 0 & 0 & 0 \end{array}\right] \left[\begin{array}{c} \dot{x}_1 \\ \hline \dot{x}_2 \\ \dot{x}_3 \end{array}\right] = \left[\begin{array}{c|cc} -1/R & 1/R & 0 \\ \hline 1 & 0 & -1 \\ 0 & 0 & 1 \end{array}\right] \left[\begin{array}{c} x_1 \\ \hline x_2 \\ x_3 \end{array}\right] - \left[\begin{array}{c} 0 \\ \hline U \\ 0 \end{array}\right]$$

Semi-discretized Stokes equation

Derivative array.

$$\left[\begin{array}{cc|cc} I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline A & B & I & 0 \\ B^T & 0 & 0 & 0 \end{array}\right] \frac{d}{dt} \left[\begin{array}{c} u_h \\ p_h \\ \dot{u}_h \\ \dot{p}_h \end{array}\right] = \left[\begin{array}{cc|cc} A & B & 0 & 0 \\ B^T & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right] \left[\begin{array}{c} u_h \\ p_h \\ \dot{u}_h \\ \dot{p}_h \end{array}\right]$$

plus boundary and initial conditions.

$$Z_2^T = \left[\begin{array}{cc|cc} 0 & I & 0 & 0 \\ -B^T & 0 & 0 & I \end{array}\right], \quad \hat{A}_2 = \left[\begin{array}{cc} B^T & 0 \\ -B^T A & -B^T B \end{array}\right].$$

Choose $T_2, Z_1^T = \left[\begin{array}{cc} U_1^T & U_2^T \end{array}\right]$ such that $\hat{A}_2 T_2 = 0$, $Z_1^T E T_2 = I_d$.

Semi-discretized Stokes.

$$\dot{u}_h = Au_h + Bp_h, \quad B^T u_h = 0,$$

Remodeled strangeness-free system

$$\begin{bmatrix} U_1^T & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{u}_h \\ \dot{p}_h \end{bmatrix} = \begin{bmatrix} U_1^T A + U_2^T B^T & U_1^T B^T \\ B^T & 0 \\ -B^T A & -B_1^T B_1 \end{bmatrix} \begin{bmatrix} u_h \\ p_h \end{bmatrix}$$

Outline

Derivative arrays, nonlinear problems

Analogous approach for $F(t,x,\dot{x}) = 0$ yields derivative array:

$$0 = F_k(t,x,\dot{x},\dots,x^{(k+1)}) = \begin{bmatrix} F(t,x,\dot{x}) \\ \frac{d}{dt}F(t,x,\dot{x}) \\ \dots \\ \frac{d^k}{dt^k}F(t,x,\dot{x}) \end{bmatrix}.$$

We set

$$\begin{aligned} M_k(t,x,\dot{x},\dots,x^{(k+1)}) &= F_{k;\dot{x},\dots,x^{(k+1)}}(t,x,\dot{x},\dots,x^{(k+1)}), \\ N_k(t,x,\dot{x},\dots,x^{(k+1)}) &= -(F_{k;x}(t,x,\dot{x},\dots,x^{(k+1)}),0,\dots,0), \\ z_k &= (t,x,\dot{x},\dots,x^{(k+1)}). \end{aligned}$$

Hypothesis: There exist integers μ, r, a, d, and v such that $\mathbf{L} = F_{\mu}^{-1}(\{0\}) \neq \emptyset$.

We have $\operatorname{rank} F_{\mu;t,x,\dot{x},\ldots,x^{(\mu+1)}} = \operatorname{rank} F_{\mu;x,\dot{x},\ldots,x^{(\mu+1)}} = r$, in a neighborhood of **L** such that there exists an equivalent system $\tilde{F}(z_{\mu}) = 0$ with a Jacobian of full row rank r. On **L** we have

1. $\operatorname{corank} F_{\mu;x,\dot{x},\ldots,x^{(\mu+1)}} - \operatorname{corank} F_{\mu-1;x,\dot{x},\ldots,x^{(\mu+1)}} = v$.
2. $\operatorname{corank} \tilde{F}_{x,\dot{x},\ldots,x^{(\mu+1)}} = a$ and there exist smooth matrix functions Z_2 (left nullspace of M_{μ}) and T_2 (right nullspace of $\hat{A}_2 = \tilde{F}_x$) with $Z_2^T \tilde{F}_{x,\dot{x},\ldots,x^{(\mu+1)}} = 0$ and $Z_2^T \hat{A}_2 T_2 = 0$.
3. $\operatorname{rank} F_{\dot{x}} T_2 = d, \quad d = \ell - a - v$, and there exists a smooth matrix function Z_1 with $\operatorname{rank} Z_1^T F_{\dot{x}} = d$.

Theorem (Kunkel/M. 2002)

The solution set **L** *forms a (smooth) manifold of dimension* $(\mu + 2)n + 1 - r$.
The DAE can locally be transformed (by application of the implicit function theorem) to a reduced DAE of the form

$$\begin{array}{rcll} \dot{x}_1 & = & G_1(t, x_1, x_3), & (d \text{ differential equations}), \\ x_2 & = & G_2(t, x_1, x_3), & (a \text{ algebraic equations}), \\ 0 & = & 0 & (v \text{ redundant equations}). \end{array}$$

The variables x_3 represent undetermined components (controls).

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{c} \\ \dot{T} \\ \dot{R} \end{bmatrix} = \begin{bmatrix} k_1(c_0 - c) - R \\ k_1(T_0 - T) + k_2 R - k_3(T - T_C) \\ R - k_3 \exp(-\frac{k_4}{T})c \end{bmatrix},$$

Suppose that T_C is given.

$$M_0 = F_{\dot{x}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \; N_0 = F_x = \begin{bmatrix} k_1 & 0 & 1 \\ k_1 & k_3 & k_2 \\ w_1 & w_2 & 1 \end{bmatrix}$$

with appropriate w_1, w_2.

$$Z_2^T = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}, \; \hat{A}_2 = \begin{bmatrix} w_1 & w_2 & 1 \end{bmatrix}, \; T_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -w_1 & -w_2 \end{bmatrix}$$

$$ET_2 = I_2, \; Z_1^T = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}.$$

Outline

Consider

$$F(t, x, \dot{x}) = 0, \quad x(t_0) = x_0$$

in the interval $\mathbb{I} = [t_0, T] \subset \mathbb{R}$.
We denote by $t_0 < t_1 < t_2 < \cdots < t_N = T$ grid-points in the interval $\mathbb{I}$ and by x_i approximations to the solution $x(t_i)$.
We discuss only fixed step-sizes, i. e., we use $t_i = t_0 + ih$, $i = 0, \ldots, N$, and $T - t_0 = Nh$.
A discretization method is given by an iteration

$$\mathfrak{X}_{i+1} = \mathfrak{F}(t_i, \mathfrak{X}_i; h),$$

where the $\mathfrak{X}_i$ are elements in some $\mathbb{R}^{\mathfrak{n}}$, together with quantities $\mathfrak{X}(t_i) \in \mathbb{R}^{\mathfrak{n}}$ representing the actual solution at t_i.

Consistency, stability, convergence

Definition

Consider a discretization method $\mathfrak{X}_{i+1} = \mathfrak{F}(t_i, \mathfrak{X}_i; h)$,

- The method is said to be consistent of order p if

$$\|\mathfrak{X}(t_{i+1}) - \mathfrak{F}(t_i, \mathfrak{X}(t_i); h)\| \leq Ch^{p+1}.$$

- It is said to be stable if there exists a vector norm $\|\cdot\|$ such that

$$\|\mathfrak{F}(t_i, \mathfrak{X}(t_i); h) - \mathfrak{F}(t_i, \mathfrak{X}_i; h)\| \leq (1 + hK)\|\mathfrak{X}(t_i) - \mathfrak{X}_i\|.$$

- It is said to be convergent of order p if

$$\|\mathfrak{X}(t_N) - \mathfrak{X}_N\| \leq Ch^p,$$

  provided that the initial value satisfies $\|\mathfrak{X}(t_0) - \mathfrak{X}_0\| \leq \tilde{C}h^p$.

Equivalence theorem

Theorem

If the discretization method

$$\mathfrak{x}_{i+1} = \mathfrak{F}(t_i, \mathfrak{x}_i; h),$$

is stable and consistent of order p, then it is convergent of order p.

Outline

A one-step method for the computation of numerical approximations x_i to the values $x(t_i)$ of a solution x of an ODE $\dot{x} = f(t, x)$ has the form

$$x_{i+1} = x_i + h\Phi(t_i, x_i; h),$$

where Φ is the so-called increment function.

The one-step method is called consistent of order p if, under the assumption that $x_i = x(t_i)$, the local discretization error $x_{i+1} - x(t_{i+1})$ satisfies

$$\|x(t_{i+1}) - x_{i+1}\| \leq Ch^{p+1},$$

with a constant C that is independent of h or equivalently

$$\|x(t_{i+1}) - x(t_i) - h\Phi(t_i, x(t_i); h)\| \leq Ch^{p+1}.$$

Setting $\mathfrak{X}_i = x_i$, $\mathfrak{X}(t_i) = x(t_i)$, and $\mathfrak{F}(t_i, \mathfrak{X}_i; h) = x_i + h\Phi(t_i, x_i; h)$, the one-step method can be seen as a general discretization method.
Since

$$
\begin{aligned}
&\|\mathfrak{F}(t_i, \mathfrak{X}(t_i); h) - \mathfrak{F}(t_i, \mathfrak{X}_i; h)\| = \\
&\qquad = \|(\mathfrak{X}(t_i) + h\Phi(t_i, \mathfrak{X}(t_i); h)) - (\mathfrak{X}_i + h\Phi(t_i, \mathfrak{X}_i; h))\| \leq \\
&\qquad \leq (1 + hK)\|\mathfrak{X}(t_i) - \mathfrak{X}_i\|,
\end{aligned}
$$

where K is the Lipschitz constant of Φ with respect to its second argument, these methods are stable without any further assumptions. Hence, consistency implies convergence of the one-step method.

Runge-Kutta methods for ODEs

The general form of an s-stage Runge-Kutta method for the solution of $\dot{x} = f(t, x)$, $x(t_0) = x_0$ is given by

$$x_{i+1} = x_i + h \sum_{j=1}^{s} \beta_j \dot{X}_{i,j},$$

where

$$\dot{X}_{i,j} = f(t_i + \gamma_j h, X_{i,j}), \quad j = 1, \ldots, s,$$

and the so-called internal stages $X_{i,j}$ are given by

$$X_{i,j} = x_i + h \sum_{l=1}^{s} \alpha_{jl} \dot{X}_{i,l}, \quad j = 1, \ldots, s.$$

The coefficients α_{jl}, β_j, and γ_j determine the particular method and are conveniently displayed in a so-called Butcher tableau

$$\begin{array}{c|c} \gamma & \mathcal{A} \\ \hline & \beta^T \end{array},$$

Conditions for the coefficients

We assume $\gamma_j = \sum_{l=1}^{s} \alpha_{jl}$ $j = 1, \ldots, s$ which implies that the method yields the same approximations to the solution x of $\dot{x} = f(t, x)$, $x(t_0) = x_0$, when we transform it to an equivalent autonomous problem by adding the trivial equation $\dot{t} = 1$, $t(t_0) = t_0$.

Theorem (Butcher 1964)

If the coefficients α_{jl}, β_j and γ_j of the Runge-Kutta method satisfy the conditions

$$
\begin{aligned}
B(p):&\quad \sum_{j=1}^{s} \beta_j \gamma_j^{k-1} &= \tfrac{1}{k}, && k = 1, \ldots, p,\\
C(q):&\quad \sum_{l=1}^{s} \alpha_{jl} \gamma_l^{k-1} &= \tfrac{1}{k}\gamma_j^k, && j = 1, \ldots, s,\ k = 1, \ldots, q,\\
D(r):&\quad \sum_{j=1}^{s} \beta_j \gamma_j^{k-1} \alpha_{jl} &= \tfrac{1}{k}\beta_l(1-\gamma_l^k), && l = 1, \ldots, s,\ k = 1, \ldots, r,
\end{aligned}
$$

with $p \leq q + r + 1$ and $p \leq 2q + 2$, then the method is consistent and hence convergent of order p.

Table: The simplest Gauß methods

$$
\begin{array}{c|c}
\frac{1}{2} & \frac{1}{2} \\
\hline
 & 1
\end{array}
\qquad
\begin{array}{c|cc}
\frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\
\frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

$$
\begin{array}{c|ccc}
\frac{1}{2} - \frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9} - \frac{\sqrt{15}}{15} & \frac{5}{36} - \frac{\sqrt{15}}{30} \\
\frac{1}{2} & \frac{5}{36} + \frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{24} \\
\frac{1}{2} + \frac{\sqrt{15}}{10} & \frac{5}{36} + \frac{\sqrt{15}}{30} & \frac{2}{9} + \frac{\sqrt{15}}{15} & \frac{5}{36} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

Radau methods

Table: The simplest Radau IIA methods

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}$$

$$\begin{array}{c|cc} \frac{1}{3} & \frac{5}{12} & -\frac{1}{12} \\ 1 & \frac{3}{4} & \frac{1}{4} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}$$

$$\begin{array}{c|ccc} \frac{4-\sqrt{6}}{10} & \frac{88-7\sqrt{6}}{360} & \frac{296-196\sqrt{6}}{1800} & \frac{-2+3\sqrt{6}}{225} \\ \frac{4+\sqrt{6}}{10} & \frac{297+169\sqrt{6}}{1800} & \frac{88+7\sqrt{6}}{360} & \frac{-2-3\sqrt{6}}{225} \\ 1 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \\ \hline & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \end{array}$$

Simple idea: Replace

$$\dot{X}_{i,j} = f(t_i + \gamma_j h, X_{i,j}), \quad j = 1, \dots, s,$$

by

$$F(t_i + \gamma_j h, X_{i,j}, \dot{X}_{i,j}) = 0, \quad j = 1, \dots, s.$$

and use the other equations

$$x_{i+1} = x_i + h \sum_{j=1}^{s} \beta_j \dot{X}_{i,j},$$

$$X_{i,j} = x_i + h \sum_{l=1}^{s} \alpha_{jl} \dot{X}_{i,l}, \quad j = 1, \dots, s.$$

as for ODEs.

Does this work?

Consider linear DAEs with constant coefficients $E\dot{x} = Ax + f(t)$, $x(t_0) = x_0$. We get

$$\begin{bmatrix} E - h\alpha_{1,1}A & -h\alpha_{1,2}A & \cdots & -h\alpha_{1,s}A \\ -h\alpha_{2,1}A & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -h\alpha_{s-1,s}A \\ -h\alpha_{s,1}A & \cdots & -h\alpha_{s,s-1}A & E - h\alpha_{s,s}A \end{bmatrix} \dot{X}_i = Z_i,$$

where

$$\dot{X}_i = \begin{bmatrix} \dot{X}_{i,1} \\ \dot{X}_{i,2} \\ \vdots \\ \dot{X}_{i,s} \end{bmatrix}, \quad Z_i = \begin{bmatrix} Ax_i + f(t_i + \gamma_1 h) \\ Ax_i + f(t_i + \gamma_2 h) \\ \vdots \\ Ax_i + f(t_i + \gamma_s h) \end{bmatrix}.$$

Existence and uniqueness conditions

- For nonsquare coefficient matrices E, A this system is not uniquely solvable for arbitrary right hand sides.
- But even in the square case, if the pair (E, A) is not regular, then the coefficient matrix is singular.
- In order to obtain a well-defined method, we must require that the pair (E, A) is regular.
- To obtain a reasonable method, it is necessary that $\mathcal{A}$ is nonsingular, which implies that we are restricted to *implicit Runge-Kutta methods*.

Theorem

Consider $N\dot{x} = x + f(t)$ *with* $\nu = \mathrm{ind}(N, I)$. *Apply a Runge-Kutta method with coefficients* $\mathcal{A}$, β, *and* γ, *and assume that* $\mathcal{A}$ *is invertible. If* $\kappa_j \in \mathbb{N}$, $j = 1, \ldots, \nu$, *exist such that*

$$\begin{aligned} \beta^T \mathcal{A}^{-k} e &= \beta^T \mathcal{A}^{-j} \gamma^{j-k}/(j-k)!, & k &= 1, 2, \ldots, j-1, \\ \beta^T \mathcal{A}^{-j} \gamma^k &= k!/(k-j+1)!, & k &= j, j+1, \ldots, \kappa_j, \end{aligned}$$

where $e = [\,1 \ \cdots \ 1\,]^T$ *of appropriate size and* $\gamma^j = [\,\gamma_1^j \ \cdots \ \gamma_s^j\,]^T$*, then the local error satisfies*

$$x(t_{i+1}) - x_{i+1} = \mathcal{O}(h^{\kappa_\nu - \nu + 2}) + \mathcal{O}(h^{\kappa_{\nu-1} - \nu + 3}) + \cdots + \mathcal{O}(h^{\kappa_1 + 1}).$$

Stiffly accurate Runge-Kutta methods

- A stiffly accurate Runge-Kutta method satisfies $\beta_j = \alpha_{sj}$ for all $j = 1, \ldots, s$.
- The Radau IIA methods are stiffly accurate by construction.
- Writing this as $\beta^T = e_s^T \mathcal{A}$ with $e_s^T = [\, 0 \ \cdots \ 0 \ 1 \,]^T$ of appropriate size, we then obtain that $\gamma_s = e_s^T \mathcal{A} e = \beta^T e$.
- Since $\beta^T e = 1$ for consistent Runge-Kutta methods, it follows that $\gamma_s = 1$. Moreover, we get that $\beta^T \mathcal{A}^{-1} e = e_s^T e = 1$, implying that κ_1 is infinite.
- Hence, these methods show the same order of consistency for regular linear DAEs with constant coefficients as for ordinary differential equations.
- For DAEs of higher index or for methods which are not stiffly accurate, however, we may have a reduction of the order.

Theorem

Consider a Runge-Kutta method with invertible $\mathcal{A}$ applied to a linear DAE with constant coefficients of the form $E\dot{x} = Ax + f(t)$, $x(t_0) = x_0$ with a regular pair (E, A) and $\nu = \mathrm{ind}(E, A)$. Furthermore, let $\kappa_j \geq j$, $j = 1, \ldots, \nu$, and

$$|1 - \beta^T \mathcal{A}^{-1} e| < 1.$$

Then the Runge-Kutta method is convergent of order

$$\min_{1 \leq j \leq \nu} \{p, \kappa_j - \nu + 2\},$$

where p is the order of the method when applied to ordinary differential equations.

What does this mean?

The order of convergence may be lower than the order of consistency. It even may happen that we loose convergence.

Example Consider again the DAE with $\mathrm{ind}(N, I) = 2$.

For this problem, the Gauß method with $s = 2$ is not convergent at all while the Radau IIA method with $s = 2$ is convergent of order two.

Methods that do not work well for constant coefficient systems cannot be expected to work for variable coefficients or nonlinear systems.

Linear systems with variable coefficients

The linear system for the stage variables has the form $(\tilde{E} - h\tilde{A})\dot{X}_i = Z_i$, with

$$\tilde{E} = \begin{bmatrix} E(t_i + \gamma_1 h) & & \\ & \ddots & \\ & & E(t_i + \gamma_s h) \end{bmatrix},$$

$$\tilde{A} = \begin{bmatrix} A(t_i + \gamma_1 h)\alpha_{11} & \cdots & A(t_i + \gamma_1 h)\alpha_{1s} \\ \vdots & & \vdots \\ A(t_i + \gamma_s h)\alpha_{s1} & \cdots & A(t_l + \gamma_s h)\alpha_{ss} \end{bmatrix}$$

and

$$Z_i = \begin{bmatrix} A(t_i + \gamma_1 h)x_i + f(t_i + \gamma_1 h) \\ \vdots \\ A(t_i + \gamma_s h)x_i + f(t_i + \gamma_s h) \end{bmatrix}.$$

Failure and ill-conditioning

- If we use for example the implicit Euler method, then $\tilde{E} = E(t_i)$ and $\tilde{A} = A(t_i)$. Thus, we need that $E(t_i) - hA(t_i)$ is invertible, which requires the pair $(E(t_i), A(t_i))$ to be regular.
- But we have seen that it may happen that the pair $(E(t), A(t))$ is singular for all t even though there exists a unique solution of the DAE. In this case the implicit Euler method fails, and higher order Runge-Kutta methods yield ill-conditioned systems.
- It is also possible that the Runge-Kutta method determines a unique numerical solution, although the given problem is not uniquely solvable at all.

Example

If we apply the Radau IIA method with $s = 2$ to the example

$$\begin{bmatrix} 0 & 0 \\ 1 & -t \end{bmatrix} \dot{x}(t) = \begin{bmatrix} -1 & t \\ 0 & 0 \end{bmatrix} x(t) + \begin{bmatrix} f_1(t) \\ f_2(t) \end{bmatrix},$$

then the coefficient matrix

$$\tilde{E} - h\tilde{A} = \left[\begin{array}{cc|cc} \frac{5}{12}h & -\frac{5}{12}h(t_i + \frac{1}{3}h) & -\frac{1}{12}h & \frac{1}{12}h(t_i + \frac{1}{3}h) \\ 1 & -(t_i + \frac{1}{3}h) & 0 & 0 \\ \hline \frac{3}{4}h & -\frac{3}{4}h(t_i + h) & \frac{1}{4}h & -\frac{1}{4}h(t_i + h) \\ 0 & 0 & 1 & -(t_i + h) \end{array}\right]$$

is invertible for all $h \neq 0$, but the condition number is $\mathcal{O}(h^{-2})$, i.e. the smaller the step-size the worse the linear system.

Example

A Runge-Kutta method may lead to an unstable recursion for the numerical solutions x_i.
Consider the linear DAE

$$\begin{bmatrix} 0 & 0 \\ 1 & \eta t \end{bmatrix} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -1 & -\eta t \\ 0 & -(1+\eta) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} f_1(t) \\ f_2(t) \end{bmatrix}$$

which is equivalent to the constant coefficient system

$$\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \dot{\tilde{x}}_1 \\ \dot{\tilde{x}}_2 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{bmatrix} + \begin{bmatrix} f_1(t) \\ f_2(t) \end{bmatrix}.$$

which has strangeness index $\mu = 1$ independent of η.

Example continued

This system has the unique solution

$$\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} f_1(t) - \eta t(f_2(t) - \dot{f}_1(t)) \\ f_2(t) - \dot{f}_1(t) \end{bmatrix}$$

without specifying initial values.
Applying the implicit Euler method gives

$$\begin{aligned} 0 &= -x_{1,i+1} - \eta t_{i+1} x_{2,i+1} + f_1(t_{i+1}), \\ \frac{1}{h}(x_{1,i+1} - x_{1,i}) + \eta t_{i+1} \frac{1}{h}(x_{2,i+1} - x_{2,i}) &= -(1+\eta) x_{2,i+1} + f_2(t_{i+1}). \end{aligned}$$

Solving the first equation for $x_{1,i}$, $x_{1,i+1}$ and inserting in the second equation

$$x_{2,i+1} = \frac{\eta}{1+\eta} x_{2,i} + \frac{1}{1+\eta}\left(f_2(t_{i+1}) - \frac{1}{h}(f_1(t_{i+1}) - f_1(t_i))\right),$$

which is divergent for $\eta < -\frac{1}{2}$.

Strangeness-free problems

- Runge-Kutta methods do not work for general DAEs.
- So we restrict the class of problems.
- In the first case, we assume semi-explicit differential-algebraic equation
$$\dot{x} = f(t, x, y), \quad 0 = g(t, x, y)$$
of index $\nu = 1$, i.e. along the given solution (x, y) the Jacobian $g_y(t, x(t), y(t))$ is nonsingular. We then show convergence results for some larger classes of Runge-Kutta methods.
- In the second case, we drop the additional assumption on the structure but treat only a restricted class of Runge-Kutta methods.

Runge-Kutta for semi-explicit DAEs

We introduce a small parameter ε to get

$$\dot{x} = f(t, x, y), \quad \varepsilon \dot{y} = g(t, x, y).$$

Applying a given Runge-Kutta method, we get

$$x_{i+1} = x_i + h \sum_{j=1}^{s} \beta_j \dot{X}_{i,j}, \quad y_{i+1} = y_i + h \sum_{j=1}^{s} \beta_j \dot{Y}_{i,j},$$

together with

$$\dot{X}_{i,j} = f(t_i + \gamma_j h, X_{i,j}, Y_{i,j}), \quad \varepsilon \dot{Y}_{i,j} = g(t_i + \gamma_j h, X_{i,j}, Y_{i,j}),$$

and

$$X_{i,j} = x_i + h \sum_{l=1}^{s} \alpha_{jl} \dot{X}_{i,l}, \quad Y_{i,j} = y_i + h \sum_{l=1}^{s} \alpha_{jl} \dot{Y}_{i,l}.$$

Setting then $\varepsilon = 0$ yields

$$\dot{X}_{i,j} = f(t_i + \gamma_j h, X_{i,j}, Y_{i,j}), \quad 0 = g(t_i + \gamma_j h, X_{i,j}, Y_{i,j})$$

Theorem

Consider an autonomous semi-explicit DAE of s-index $\nu = 0$ *together with consistent initial values* (x_0, y_0) *due to* $0 = g(x_0, y_0)$*. Apply a Runge-Kutta method given by with invertible coefficient matrix* $\mathcal{A}$*. Assume that it has order p for ODEs and that it satisfies condition* $C(q)$ *with* $p \geq q + 1$*, and let* $\varrho = 1 - \beta^T \mathcal{A}^{-1} e$*. If* $|\varrho| \leq 1$*, then the global error satisfies*

$$\|x(t_N) - x_N\| = \mathcal{O}(h^k).$$

1. *If* $\varrho = 0$*, then* $k = p$*.*
2. *If* $-1 \leq \varrho < 1$*, then* $k = \min\{p, q + 1\}$*.*
3. *If* $\varrho = 1$*, then* $k = \min\{p - 1, q\}$*.*

If $|\varrho| > 1$*, then the method is not convergent.*

Runge-Kutta for strangeness free DAEs

Theorem

The Radau IIA methods applied to regular strangeness-free DAEs are convergent of order $p = 2s - 1$.

- All presented convergence results are based on the assumption that we use a constant stepsize.
- For real-life applications, however, a sophisticated strategy for the adaption of the stepsize during the numerical solution of the problem is indispensable.
- In the case of semi-explicit DAEs of index $\nu = 1$ or regular strangeness-free problems, it is possible to use the same techniques as in the case of ordinary differential equations.
- However, when discretizing higher index systems, changes of the stepsize may lead to undesired effects.

Outline

Linear multi-step methods for ODEs

- Multi-step methods use previous approximations $x_{i-1}, \ldots, x_{i-k}$ for the approximation x_i to $x(t_i)$.
- For real α_l and β_l for $l = 0, \ldots, k$, a linear multi-step method for the numerical solution of an ODE $\dot{x} = f(t, x)$ is given by

$$\sum_{l=0}^{k} \alpha_{k-l} x_{i-l} = h \sum_{l=0}^{k} \beta_{k-l} f(t_{i-l}, x_{i-l}).$$

- In order to fix x_i at least for sufficiently small stepsizes h, we require that $\alpha_k \neq 0$. In addition, we assume that $\alpha_0^2 + \beta_0^2 \neq 0$.
- We must provide $x_0, \ldots, x_{k-1}$ to initialize the iteration.
- The α_l and β_l define the characteristic polynomials

$$\varrho(\lambda) = \sum_{l=0}^{k} \alpha_l \lambda^l, \quad \sigma(\lambda) = \sum_{l=0}^{k} \beta_l \lambda^l$$

of the multi-step method.

General discretization method

Setting

$$\mathfrak{x}_i = \begin{bmatrix} x_{i+k-1} \\ x_{i+k-2} \\ \vdots \\ x_i \end{bmatrix}, \quad \mathfrak{x}(t_i) = \begin{bmatrix} x(t_{i+k-1}) \\ x(t_{i+k-2}) \\ \vdots \\ x(t_i) \end{bmatrix},$$

we get a general discretization method.

Consistency and stability

- The multi-step method is called consistent of order p if

$$\sum_{l=0}^{k} \alpha_{k-l} x(t_{i-l}) - h \sum_{l=0}^{k} \beta_{k-l} \dot{x}(t_{i-l}) = \mathcal{O}(h^{p+1})$$

  for all sufficiently smooth functions x.
- A multi-step method is called stable if there exists a vector norm such that in the associated matrix norm

$$\|\mathcal{C}_\alpha \otimes I_n\| \leq 1,$$

  where

$$\mathcal{C}_\alpha = \begin{bmatrix} -\alpha_{k-1} & \cdots & -\alpha_1 & -\alpha_0 \\ 1 & & & \\ & \ddots & & \\ & & 1 & \end{bmatrix}$$

  is the companion matrix given by $\alpha_0, \ldots, \alpha_{k-1}, \alpha_k = 1$.

Consistency theorem

Theorem

If the coefficients α_l and β_l, $l = 1, \ldots, k$, of the multi-step method satisfy the conditions

$$\sum_{l=0}^{k} \alpha_l l^q = q \sum_{l=0}^{k} \beta_l l^{q-1}, \quad q = 0, \ldots, p,$$

with the convention that the right hand side vanishes for $q = 0$ and that $0^0 = 1$, then the method is consistent of order p.

In order to get consistency of order at least $p = 1$, we must therefore require

$$\varrho(1) = 0, \quad \dot{\varrho}(1) = \sigma(1).$$

Stability and Convergence Theorem

Theorem

Suppose that the characteristic polynomial ϱ of the multi-step method satisfies the so-called root condition given by:

1. *The roots of ϱ lie in the closed unit disk.*
2. *The roots of ϱ with modulus one are simple.*

Then the multi-step method is stable.

Theorem

Suppose that the coefficients α_l and β_l, $l = 1, \ldots, k$, of the multi-step method satisfy the consistency condition with order p and the root condition, then the multi-step method is convergent of order p.

In the context of DAEs, the most popular linear multi-step methods are the so-called BDF methods. The abbreviation BDF stands for *backward differentiation formulae*.
These methods are obtained by setting

$$\beta_0 = \cdots = \beta_{k-1} = 0, \quad \beta_k = 1,$$

and choosing α_l, $l = 1, \ldots, k$, to satisfy the consistency condition with p as large as possible. We can achieve $p = k$.

Table: The simplest BDF methods

α_{k-l}	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$	$l=5$	$l=6$
$k=1$	1	-1					
$k=2$	$\frac{3}{2}$	-2	$\frac{1}{2}$				
$k=3$	$\frac{11}{6}$	-3	$\frac{3}{2}$	$-\frac{1}{3}$			
$k=4$	$\frac{25}{12}$	-4	3	$-\frac{4}{3}$	$\frac{1}{4}$		
$k=5$	$\frac{137}{60}$	-5	5	$-\frac{10}{3}$	$\frac{5}{4}$	$-\frac{1}{5}$	
$k=6$	$\frac{147}{60}$	-6	$\frac{15}{2}$	$-\frac{20}{3}$	$\frac{15}{4}$	$-\frac{6}{5}$	$\frac{1}{6}$

Theorem

The BDF methods are stable only for $1 \leq k \leq 6$.

Use the difference operator

$$D_h x_i = \frac{1}{h} \sum_{l=0}^{k} \alpha_{k-l} x(t_{i-l}).$$

Then BDF methods for DAEs have the form

$$F(t_i, x_i, D_h x_i) = 0, \quad D_h x_i = \frac{1}{h} \sum_{l=0}^{k} \alpha_{k-l} x_{i-l}.$$

Theorem

Let (E, A) be regular with $\nu = \mathrm{ind}(E, A)$. Then the BDF methods with $1 \leq k \leq 6$, applied to the system $E\dot{x} = Ax + f(t)$, $x(t_0) = x_0$, are convergent of order $p = k$.

BDF for linear DAEs II

If we discretize $E(t)\dot{x} = A(t)x + f$ by a BDF method, then we obtain

$$E(t_i)\frac{1}{h}\sum_{l=0}^{k}\alpha_{k-l}x_{i-l} = A(t_i)x_i + f(t_i),$$

or, equivalently, by collecting the terms in x_i,

$$(\alpha_k E(t_i) - hA(t_i))x_i = hf(t_i) - E(t_i)\sum_{l=1}^{k}\alpha_{k-l}x_{i-l}.$$

It follows that a unique numerical solution x_i exists if and only if the matrix $\alpha_k E(t_i) - hA(t_i)$ is invertible. This is only possible if the matrix pair $(E(t_i), A(t_i))$ is regular.

We get the same problems as for Runge-Kutta methods.

BDF for semi-explicit s-free DAEs

Theorem

Consider an BDF method of order p applied to a semi-explicit strangeness-free DAE. Suppose that ϱ as well as σ satisfy the root condition. Then the method is convergent of order p.

BDF for s-free DAEs

Theorem

The BDF discretization for a general regular strangeness-free DAE is convergent of order $p = k$ for $1 \leq k \leq 6$ provided that the initial values $x_0, \dots, x_{k-1}$ are consistent.

There are no difficulties to supply BDF methods with a stepsize control and oorder control.

Where are we?

- We have shown that every nonlinear DAE that satisfies the Hypothesis can be turned into a strangeness-free DAE.
- For general strangeness-free DAEs, certain classes of Runge-Kutta and multi-step methods work as for ODEs.
- So if we remodel the DAE in a strangeness-free way, we can solve them nicely.

Consistent initial values are obtained by solving $F_\mu(t_0, x, \dot{x}, \ldots, x^{(\mu+1)}) = 0$ at t_0 for the algebraic variable $(x, \dot{x}, \ldots, x^{(\mu+1)})$.

For the integration of the DAE, e.g. with BDF methods, the system

$$\begin{aligned} F_\mu(t_0 + h, x, \dot{x}, \ldots, x^{(\mu+1)}) &= 0, \\ \tilde{Z}_1^T F(t_0 + h, x, D_h x) &= 0 \end{aligned}$$

is solved for $(x, \dot{x}, \ldots, x^{(\mu+1)})$.

Here, $\tilde{Z}_1$ denotes a suitable approximation of Z_1 at the desired solution, and

$$D_h x_i = \frac{1}{h} \sum_{l=0}^{k} \alpha_l x_{i-l},$$

is the discretization by BDF or other finite difference operators.

Theorem (Kunkel/M. 2002)

Let F satisfy the nonlinear Hypothesis.
Then, the occurring Jacobians of the system have full row rank at the solution provided the step-size h is sufficiently small and the approximation $\tilde{Z}_1$ is sufficiently good.

- *Simplified Gauss-Newton method can be used to solve the nonlinear systems at every integration step.*
- *The order and convergence properties are the same as for ODEs.*
- *Method can be implemented by using local computations only.*

Outline

Several production codes were derived.

- Production code GELDA Kunkel/M./Rath/Weickert 1998 (linear variable coefficients), uses BDF and Runge-Kutta discretization.
- Production code GENDA (nonlinear regular), Kunkel/M./Seufer 2002 based on BDF.
- Matlab code SOLVEDAE (nonlinear), Kunkel/Mehrmann/Seidel 2005.
- Special multi-body code GEOMS Steinbrecher 2006.
- Circuit codes, joint with NEC, Bächle, Ebert, 2006.

Numerical Example: Truck

Consider the nonlinear model of a truck which is a constrained multibody system written in the Euler–Lagrange equations

$$\begin{aligned} \dot{p} &= v \\ M(p,t)\dot{v} &= f(p,v,t) - G^T(p,t)\lambda \\ 0 &= g(p,t). \end{aligned}$$

$M(p,t)$ stands for the symmetric positive definite mass matrix, the vector $f(p,v,t)$ denotes the applied forces and $G(p,t) := \frac{\partial}{\partial p} g(p,t)$ is the Jacobian of the holonomic constraints $g(p,t)$. The system has strangeness index 2 and dimension 23. $\rightarrow$ film.

Numerical Example: Ball on surface

Consider the nonlinear model of a ball rolling on a parabolic surface $\rightarrow$ film.

Where is the catch?

- This is a general purpose approach for the analysis and numerical solution of general over- or underdetermined DAEs.
- At every integration step the derivative array has to be formed, the projection matrices and the Jacobians have to be computed.
- Method is in this form not feasible for large scale problems arising from coupled systems of PDEs.
- Explicit knowledge about the structure of the problem is not used.
- Analytical information about the manifolds and the contraints must be incorporated.
- The specific structure of the problem must be used to make the approach efficient.

New modeling paradigm!

- Include all possible constraints into the mathematical model.
- Identify all equations that need to be differentiated, if possible based on physical observations, or structural arguments.
- Create reduced derivative array by adding all necessary derivatives to system.
- Apply strangeness-index concept to determine projectors to strangeness-free form.
- Do this first seperately with all submodels.
- Then identify problems arising due to coupling and reduce the index. Network based approach Bächle/Ebert 2006
- **If possible, model directly in strangeness-free form.**