Chapter 4  Numerical solution of stiff and differential-algebraic equations

4.1  Characteristics of stiff systems

The solution has components with extremely different growth properties.

Example:

\[
\begin{align*}
2 u'(x) &= (q_1 + q_2) u(x) + ((q_1 - q_2) v(x) , \ u(a) = 2 ,
2 v'(x) &= (q_1 - q_2) u(x) + ((q_1 + q_2) v(x) , \ v(a) = 0
\end{align*}
\]

with the solution

\[
\begin{align*}
u(x) &= \exp(q_1(x-a)) + \exp(q_2(x-a)) , \ v(x) = \exp(q_1(x-a)) - \exp(q_2(x-a)) .
\end{align*}
\]

The explicit Euler method provides the approximations

\[
\begin{align*}
u_j &= (1 + h q_1)^j + (1 + h q_2)^j , \ v_j = (1 + h q_1)^j - (1 + h q_2)^j .
\end{align*}
\]

If \( Req_1 < 0 \), \( Req_2 < 0 \) and the approximations should behave in the same way as the solution, the following two conditions must be satisfied simultaneously:

\[
|1 + h q_1| < 1 , \ |1 + h q_2| < 1 .
\]
In case $\text{Req}_2 < \text{Req}_1 < 0$, the requirements

$$|1 + h q_1| < 1, \quad |1 + h q_2| < 1$$

imply the condition

$$(\bullet) \quad h |q_2| < 2.$$ 

The components of $u$ and $v$ associated with $q_2$ decay faster than the components associated with $q_1$, in particular, if $\text{Req}_2 \ll \text{Req}_1$.

After an initial phase until a sufficient decay of $\exp(q_2(x - a))$ compared to $\exp(q_1(x - a))$, one should expect that the accuracy of the approximations and hence the step size $h$ is only determined by the component associated with $q_1$, if only the component associated with $q_2$ is integrated stably, i.e., such that it does not increase. However, this does not hold true for the explicit Euler method. Here, the step size has always to be chosen according to $(\bullet)$, which is much too small from the point of view of accuracy.
On the other hand, the application of the implicit Euler method gives:

\[
\begin{align*}
\phantom{=} u_j &= \frac{1}{(1 - h q_1)^j} + \frac{1}{(1 - h q_2)^j}, \quad j \geq 0, \\
\phantom{=} v_j &= \frac{1}{(1 - h q_1)^j} - \frac{1}{(1 - h q_2)^j}, \quad j \geq 0.
\end{align*}
\]

Without any restriction of the step size \( h \), the approximations decay for increasing \( j \).

**Consequence:** We need special integrators for stiff systems.
4.2 One step methods for stiff systems

4.2.1 Linear stability theory

In case of linear systems \( y' = Ay \), the growth properties of the solutions are determined by the eigenvalues \( \lambda \in \sigma(A) \). In case of nonlinear systems \( y' = f(y) \), local information is obtained by the eigenvalues of the Jacobi matrix \( J_f(y^*) := f'_y(y^*) \).

**Definition 4.1 Lokal and global contractivity**

Assume that \( f \in C^1(D) \), \( D \subset \mathbb{R}^d \), and that \( \langle \cdot, \cdot \rangle \) is an inner product on \( \mathbb{R}^d \) with associated norm \( \| \cdot \| \). Moreover, let \( y^* \in C(I) \) and \( A := f'_y(y^*) \). If

\[
\langle u, Au \rangle \leq \mu(A) \| u \|^2 , \quad u \in \mathbb{R}^d ,
\]

the quantity \( \mu(A) \) is called the local, one-sided Lipschitz constant. If \( \mu(A) < 0 \), the system \( y' = f(y) \) is said to be locally contractive.

If there exists \( \bar{\mu} \in \mathbb{R} \) such that

\[
\langle f(u) - f(v), u - v \rangle \leq \bar{\mu} \| u - v \|^2 , \quad u, v \in \mathbb{R}^d ,
\]

the quantity \( \bar{\mu} \) is called the global, one-sided Lipschitz constant. If \( \bar{\mu} < 0 \), the system \( y' = f(y) \) is said to be globally contractive.
Theorem 4.2  Growth properties of nonlinear autonomous systems

Under the assumption

\[ \langle f(u) - f(v), u - v \rangle \leq \bar{\mu} \|u - v\|^2 , \quad u, v \in \mathbb{R}^d , \]

for \( x \in I \) there holds

\[ \|u(x) - v(x)\| \leq \exp(\bar{\mu}(x - a)) \|u(a) - v(a)\| . \]

Proof: Straightforward application of Gronwall’s lemma.

Theorem 4.3  Ljapunov stability

Assume that \( A \in \mathbb{R}^{n \times n} \) is a matrix whose eigenvalues \( \lambda(A) \in \sigma(A) \) satisfy

\[ \text{Re} \lambda(A) < 0 . \]

Then, there exist constants \( c \geq 0 \) and \( \mu \leq 0 \) such that the solution \( y \in C^1(I) \) of the initial value problem \( y' = Ay , \quad y(a) = \alpha \), satisfies

\[ \|y(x)\| \leq c \exp(\mu(x - a)) , \quad x \in I . \]

Proof: Orthogonal transformation of \( A \) to Schur’s normal form and recursive solution of the transformed initial value problem.
Affine covariance of autonomous systems

Consider the initial value problem

\[(AWP)_1 \quad y'(x) = f(y(x)) \quad , \quad x \in I , \]

\[(AWP)_2 \quad y(a) = \alpha . \]

If \(B\) is a non singular \(n \times n\) matrix such that \(B_x \equiv 0\), the affine transformation

\[y \mapsto B y =: \bar{y}\]

of the variable \(y\) results in the transformed initial value problem

\[(AWP)'_1 \quad \bar{y}' = \bar{f}(\bar{y}(x)) \quad , \quad x \in I , \]

\[(AWP)'_2 \quad \bar{y}(a) = B\alpha , \]

where \(\bar{f}(\bar{y}) := Bf(B^{-1}\bar{y})\). The existence and uniqueness theorem provides the relationship

\[\bar{y} = By , \]

which is referred to as the affine covariance of the autonomous system.
Definition 4.4 Affine covariance of numerical integrators
A numerical integrator for the solution of an initial value problem for a system of first order ordinary differential equations is called affine covariant, if there holds:
If $B$ is a non singular $n \times n$ matrix such that $Bx \equiv 0$ and $y_h \in C(I_h)$ is an approximation of the solution $y \in C^1(I)$ of the initial value problem, obtained by the integrator, then $\bar{y}_h = By_h$ is an approximation of $\bar{y} = By$.

Consequence of affine covariance: scalar test equation
The local stability of the initial value problem $(AWP)_1, (AWP)_2$ is determined by the eigenvalues of the Jacobi matrix $f_y$. The spectrum of the Jacobi matrix is invariant with respect to similarity transformations

$$f_y \mapsto B f_y B^{-1}.$$  

If $A := f_y$ is diagonalizable, there exists a non singular matrix $B$ such that

$$B A B^{-1} = \text{diag}(\lambda_1, ..., \lambda_n),$$

where $\lambda_i \in \sigma(A), 1 \leq i \leq n$. Due to the affine covariance it is sufficient to consider the scalar test equation

$$(T) \quad y'(x) = \lambda y(x), \quad x > 0, \quad y(0) = 1 \quad (\lambda \in C).$$
The solution of the scalar test equation \((T)\) is given by

\[
y(x) = \exp(\lambda x) \quad , \quad x \geq 0.
\]

Setting \(z := \lambda x, z \in \mathbb{C}\), the restriction of \(y\) to a uniform grid of step size \(h > 0\) results in the following characterization of the stability of the solution of the scalar test equation:

\[
\begin{align*}
(i) \quad & \quad \text{Re } z < 0 \implies |y(h)| = |\exp(z)| < 1, \\
(ii) \quad & \quad \text{Re } z = 0 \implies |y(h)| = |\exp(z)| = 1, \\
(iii) \quad & \quad \text{Re } z > 0 \implies |y(h)| = |\exp(z)| > 1.
\end{align*}
\]

Going to the limit \(z \to \infty\), we see that in \(z = \infty\) there is an essential singularity of the solution of the test equation:

\[
\begin{align*}
(i) \quad & \quad \text{Re } z < 0 \implies y(h) \to 0 \quad (z \to \infty), \\
(ii) \quad & \quad \text{Re } z = 0 \implies |y(h)| = 1 \quad (z \to \infty), \\
(iii) \quad & \quad \text{Re } z > 0 \implies |y(h)| \to \infty \quad (z \to \infty).
\end{align*}
\]
Behavior of solutions of classical one-step methods applied to the test equation

a) Explicit Euler method

\[ y_1 = y_0 + h \lambda y_0 = (1 + h \lambda) = 1 + z \implies y_1 \to \infty \quad (z \to \infty). \]

b) Implicit Euler method

\[ y_1 = y_0 + h \lambda y_1 \implies y_1 = \frac{1}{1 - z} \implies y_1 \to 0 \quad (z \to \infty). \]

c) Implicit trapezoidal rule

\[ y_1 = y_0 + \frac{h}{2} \lambda (y_1 + y_0) \implies y_1 = \frac{1 + z/2}{1 - z/2} \implies |y_1| = 1 \quad (z \to \infty). \]
General implicit one-step methods
Implicit one-step methods lead to rational functions:

$$y_1 = R_{\ell m}(z) y_0 = \frac{P_\ell(z)}{Q_m(z)} y_0,$$

where $R_{\ell m}(z)$ is an approximation of $\exp(z)$.

Definition 4.5 Padé approximation of the exponential function
Let $\ell, m \in \mathbb{N}_0$ and $P_\ell, Q_m$ polynomials of degree $\ell$ resp. $m$. If

$$\exp(z) Q_m(z) - P_\ell(z) = O(|z|^{|\ell+m+1|}) \quad (z \to 0),$$

the rational function

$$R_{\ell m}(z) = \frac{P_\ell(z)}{Q_m(z)}$$

is called a Padé approximation of $\exp(z)$ of index $(m, \ell)$.

The stability region of an implicit one-step method with $R = R_{\ell m}$ is given by

$$G := \{ z \in \mathbb{C} \mid |R(z)| \leq 1 \}.$$
Stability regions for numerical integrators

The stability region (in the sense $y \to 0$ as $z \to \infty$) of the analytical solution $y = \exp(z)$ of the test equation is the complex hyperplane

$$G_A = C_- := \{ z \in \mathbb{C} \mid \text{Re } z \leq 0 \}.$$

Natural requirement for the stability region of a numerical integrator:

$$(\star) \quad G = C_- .$$

Consequences of $(\star)$ with regard to Padé approximations:

Since the imaginary axis $\text{Re } z = 0$ corresponds to the sphere $|R(z)| = 1$, we must have

$$(\diamond) \quad |R(z)| = 1 \text{ for } \text{Re } z = 0 .$$

Since $(\diamond)$ must be satisfied for $\text{Im } z \to \pm \infty$ as well,

$$R(z) = \frac{P_\ell(z)}{Q_\ell(z)} \quad (\text{diagonal Padé approximation}).$$
Since $\bar{z} = -z$ for $\Re z = 0$, it follows that

$$1 = |R(z)|^2 = R(z) \bar{R}(z) = R(z) R(\bar{z}) = R(z) R(-z).$$

In view of $R(z) = P_\ell(z)/Q_\ell(z)$ this implies

$$P_\ell(z) P_\ell(-z) = Q_\ell(z) Q_\ell(-z) \implies P_\ell(-z) = Q_\ell(z).$$

**Example:** Implicit trapezoidal rule

$$P_1(z) = 1 + \frac{z}{2}, \quad Q_1(z) = 1 - \frac{z}{2} = P_1(-z) \implies R(\infty) = -1.$$

In general: **Oscillatory behavior** due to $R(\infty) = (-1)^\ell$. 
A-stability, L-stability and super stability

Dahlquist’s condition [Dahlquist (1963)]:
If the analytical solution is decreasing, this should be reflected by the numerical approximation.

Definition 4.6  A-stability
A one-step method with Padé approximation \( R = R(z) \) is called A-stable, if

\[
C_- \subset G .
\]

Lemma 4.7  A-stability of diagonal and subdiagonal Padé approximations
('Ehle’s conjecture') [Hairer, Norsett, Wanner (1978)]
One-step methods with Padé approximations of index \((m, \ell)\), \(\ell \leq m \leq \ell + 2\), are A-stable.
The implicit trapezoidal rule is A-stable, but \( R(z) \to -1 \) as \( z \to \infty \). This motivates:

Definition 4.8  L-stability
An A-stable one-step method is called L-stable, if

\[
R(z) \to 0 \quad \text{as} \quad \Re z \to -\infty .
\]

Lemma 4.9  L-stability of subdiagonal Padé approximations
One-step methods with Padé approximations of index \((\ell + 1, \ell)\) are L-stable.
Definition 4.10 Super stability
An L-stable one-step method is called super stable, if
\[ C_- \subset G , \quad \text{i.e.,} \quad G \setminus C_- \neq \emptyset . \]

Example: Implicit Euler method
Stability region:
\[ G := \{ z \in \mathbb{C} \mid |z - 1| > 1 \} . \]

Definition 4.11 $A(\alpha)$-stability [Widlund (1967)]
A one-step method with Padé approximation $R = R(z)$ is called $A(\alpha)$-stable, if
\[ G = G(\alpha) = \{ z \in \mathbb{C} \mid |\arg z - \pi| \leq \alpha \} . \]

Example: BDF methods (see below)
4.3 Implicit and semi-implicit Runge-Kutta methods

Implicit s-stage Runge-Kutta method:

Setting $c_i := \sum_{j=1}^{s} a_{ij}$, $1 \leq i \leq s$:

$$
k_1 = h f(x_k + c_1 h, y_k + \sum_{j=1}^{s} a_{1j} k_j), \quad c_1 \mid a_{11} \cdots a_{1s}
$$

$$
\cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \·

$$

$$
k_s = h f(x_k + c_s h, y_k + \sum_{j=1}^{s} a_{sj} k_j), \quad c_s \mid a_{s1} \cdots a_{ss}
$$

$$
y_{k+1} = y_k + \sum_{j=1}^{s} b_j k_j, \quad b_1 \cdots b_s
$$

Butcher scheme
Implicit Runge-Kutta methods require the solution of a nonlinear system.

Setting \( k_i = h \, f(x_k + c_i h, g_i) \), it follows that

\[
g_i = y_k + h \sum_{j=1}^{s} a_{ij} \, f(x_k + c_j h, g_j), \quad 1 \leq i \leq s.
\]

**Linear stability theory:**

Application to the scalar test equation yields (with \( A := (a_{ij})_{i,j=1}^{s} \)):

\[
\begin{pmatrix}
g_1 \\
\vdots \\
g_s
\end{pmatrix} = \begin{pmatrix} 1 \\
\vdots \\
1
\end{pmatrix} y_k + h \lambda \begin{pmatrix} 1 \\
\vdots \\
1
\end{pmatrix} A \begin{pmatrix} g_1 \\
\vdots \\
g_s
\end{pmatrix} \quad \Rightarrow \quad (I_s - z A) \begin{pmatrix} y_k \\
\vdots \\
z g
\end{pmatrix} \quad \Rightarrow
\]

If \( (I_s - z A) \) is non singular:

\[
y_{k+1} = y_k + b^T k = \left[ 1 + z \, b^T (I_s - z A)^{-1} e \right] y_k.
\]
The representation
\[ y_{k+1} = y_k + b^T k = \left[ 1 + z b^T (I_s - z A)^{-1} e \right] y_k. \]
gives rise to the stability function:
\[ R_s(z) = 1 + b^T \left( \frac{1}{z} (I_s - A) \right) e. \]

If \( A \) is non singular:
\[ R_s(\infty) = 1 - b^T A^{-1} e. \]

L-stability: \( R_s(\infty) = 0 \)

Example: 'Fehlberg-trick' for implicit Runge-Kutta methods
\[ a_{sj} = b_j , \quad 1 \leq j \leq s \quad \Rightarrow \]
\[ c_s = \sum_{j=1}^{s} a_{sj} = \sum_{j=1}^{s} b_j = 1 \quad \Rightarrow \]
\[ b^T = e_s^T A , \quad \text{where} \quad e_s := (0, \ldots, 0, 1)^T \quad \Rightarrow \]
\[ R_s(\infty) = 1 - e_s^T A A^{-1} e = 0. \]
Solution of the nonlinear system by a simplified Newton method

\[ G(g_1, \ldots, g_s) = \begin{cases} g_1 - y_k - h \sum_{j=1}^{s} a_{1j} f(x_k + c_1 h, g_j) \\ g_s - y_k - h \sum_{j=1}^{s} a_{sj} f(x_k + c_s h, g_j) \end{cases} = 0. \]

For the Jacobi matrix at \( g_i = y_k \), we obtain:

\[ \frac{\partial G_i}{\partial g_\ell} |_{g_\ell = y_k} = \delta_i \ell I_d - h a_{i\ell} f_y(x_k + c_i h, g_\ell) |_{g_\ell = y_k} = \delta_i \ell I_d - h a_{i\ell} f_y(x_k, y_k) + O(h^2). \]

It follows that

\[ J = \begin{bmatrix} I_d - ha_{11} A & -ha_{12} A & \cdots & -ha_{1s} A \\ -ha_{21} A & I_d - ha_{22} A & \cdots & -ha_{2s} A \\ \vdots & \ddots & \ddots & \vdots \\ -ha_{s1} A & -ha_{s2} A & \cdots & I_d - ha_{ss} A \end{bmatrix}. \]

Since \( J |_{h=0} = I \), we find that \( J \) is regular for sufficiently small \( h > 0 \).
Simplified Newton method:

Choose $g^{(0)} = (g_1^{(0)}, ..., g_s^{(0)})^T$ with $g_i^{(0)} = y_k$, $1 \leq i \leq s$. Then, for $k = 0, 1, 2, ...$ compute:

$$J \Delta g^{(k)} = -G(g^{(k)}) ,$$

$$g^{(k+1)} = g^{(k)} + \Delta g^{(k)} .$$
Simplifications:

a) DIRK (Diagonally Implicit Runge-Kutta)

$$
\begin{array}{c|cccc}
  c_1 & a_{11} & 0 & 0 & \cdots & 0 \\
  c_2 & a_{21} & a_{22} & 0 & \cdots & 0 \\
  \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\
  c_s & a_{s1} & a_{s2} & a_{s3} & \cdots & a_{ss} \\
  b_1 & b_2 & b_3 & \cdots & b_s \\
\end{array}
$$

LR decomposition of $s$ matrices of the form

$$I_d - h a_{ij} A = L_i R_i , \quad 1 \leq i \leq s .$$
Simplifications:

b) SDIRK (Singly Diagonally Implicit Runge-Kutta)

\[
\begin{array}{c|cccc}
  c_1 & \gamma & 0 & 0 & \cdots & 0 \\
  c_2 & a_{21} & \gamma & 0 & \cdots & 0 \\
  . & . & . & . & . & . \\
  c_s & a_{s1} & a_{s2} & a_{s3} & \cdots & \gamma \\
  b_1 & b_2 & b_3 & \cdots & b_s \\
\end{array}
\]

LR decomposition of only one matrix:

\[ I_d - h \gamma A = L R. \]
Semi-implicit Runge-Kutta methods:
Implementation of only one Newton iteration:

\[
J \Delta g^{(0)} = - G(g^{(0)}) ,
\]
\[
g^{(1)} = g^{(0)} + \Delta g^{(0)} ,
\]

where \( g^{(0)} = (g^{(0)}_1, ..., g^{(0)}_s)^T \) with \( g^{(0)}_i = y_k , \ 1 \leq i \leq s. \)

Rosenbrock methods:
Construction for the example of an autonomous system:
Idea: Additional consideration of \( f_y(y_k) \) in the order conditions

\[
k_i = h f(y_k) + \sum_{j=1}^{s} a_{ij} k_j + h f_y(y_k) \sum_{j=1}^{s} \bar{a}_{ij} k_j , \ 1 \leq i \leq s ,
\]
\[
y_{k+1} = y_k + \sum_{j=1}^{s} b_j k_j .
\]

Embedded Rosenbrock methods of type \((3,4)\) with step size control:
GRK4T \ [Kaps/Rentrop (1979)]
W methods [Wolfbrandt/Wanner]

\[
  k_i = f(y_k + h \sum_{j=1}^{i-1} a_{ij} k_j) + h A \sum_{j=1}^{i-1} \bar{a}_{ij} k_j + h A \gamma k_i, \quad 1 \leq i \leq s,
\]

\[
y_{k+1} = y_k + h \sum_{j=1}^{s} b_j k_j,
\]

where \( A := f_y(y_k) \).

Interpretation as an SDIRK method with only one Newton iteration
(close relationship with semi-implicit Runge-Kutta methods)
4.4 Multi-step methods for stiff systems of differential equations

4.4.1 Linear stability theory

Consider the linear $m$-step method

\[
(LMSV) \quad \sum_{k=0}^{m} \alpha_k y_{j+k} = h \sum_{k=0}^{m} \beta_k f(x_{j+k}, y_{j+k})
\]

with the characteristic polynomials

\[
\rho(z) = \sum_{k=0}^{m} \alpha_k z^k, \quad \sigma(z) = \sum_{k=0}^{m} \beta_k z^k.
\]

Application to the scalar test equation

\[
y'(x) = \lambda y(x), \quad x > 0, \quad y(0) = 1
\]

results in (set $z := \lambda h \in C$):

\[
\sum_{k=0}^{m} (\alpha_k - \beta_k z) y_{j+k} = 0.
\]

The ansatz $y_\ell = z^\ell$ leads to characteristic equation

\[
\rho(z) - z \sigma(z) = 0.
\]
Lemma 4.12 Stability region of linear multi-step methods
Assume that $\xi_i = \xi_i(z), 1 \leq i \leq m$, are the roots of the characteristic equation (CG). Then, the stability region of (LMSV), applied to the scalar test equation, is given by

$$G = \{ z \in \mathbb{C} \mid |\xi_i(z)| \leq 1, 1 \leq i \leq m, \text{ and } \xi_i(z) \text{ simple, if } |\xi_i(z)| = 1 \}.$$  

Definition 4.13 Root locus
Parameterizing $\partial G$ according to

$$|\xi| = 1 \rightarrow \xi = \exp(i\varphi), \quad \varphi \in [0, 2\pi),$$

the resulting curve

$$\Gamma := \{ z \in \mathbb{C} \mid z = \frac{\rho(\exp(i\varphi))}{\sigma(\exp(i\varphi))}, \varphi \in [0, 2\pi) \}$$

is called root locus.

Remark 4.14 Stability region and root locus
Since $\partial G$ only contains simple roots, there holds

$$\partial G \subset \Gamma.$$
Study of A-stability

Example 4.15 Explicit midpoint rule

\[ y_{k+2} = y_k + 2 h \lambda y_{k+1} = y_k + 2 z y_{k+1} \implies \]
\[ \rho(\xi) = \xi^2 - 1 , \quad \sigma(\xi) = 2 \xi \implies \]
characteristic equation:

\[ \xi^2 - 2 z \xi - 1 = 0 \implies \]
\[ \xi_{1,2} = z \pm \sqrt{1 + z^2} \]

The root locus is given as follows:

\[ z = \frac{\rho(\exp(i\varphi))}{\sigma(\exp(i\varphi))} = \frac{\exp(2i\varphi) - 1}{2 \exp(i\varphi)} = \frac{1}{2} \left[ \exp(i\varphi) - \exp(-i\varphi) \right] = i \sin \varphi \implies \]
\[ \Gamma = \{ z \in \mathbb{C} \mid z = i\tau , \ \tau \in [-1,1] \} . \]

Multiple roots:

\[ \xi_1 = \xi_2 \iff 1 + z^2 = 0 \iff z = \pm i . \]

Stability region:

\[ G = \partial G = \{ z \in \mathbb{C} \mid z = i\tau , \ \tau \in (-1,1) \} . \]

Since \( C_\leftarrow \not\in G \implies \) no A-stability.
**Theorem 4.16 Second Dahlquist barrier [Dahlquist (1963)]**

A consistent, A-stable linear multi-step method necessarily is implicit and has an order of consistency $p \leq 2$ with normalized error constant $C^* := C/\sigma(1) \leq -\frac{1}{12}$.

The **implicit trapezoidal rule** is the only A-stable method with $p = 2$, $C^* = -\frac{1}{12}$ and $\alpha_m = 1$.

#### 4.4.2 BDF methods

$$\sum_{k=1}^{m} \frac{1}{k} \nabla^k y_{j+m} = h f(x_{j+m}, y_{j+m}) , \quad 0 \leq j \leq N - m .$$

**Stability properties:**

(i) A-stability for $m = 1, 2$ ($m = 1$ : implicit Euler)

(ii) $A(\alpha)$-stability for $3 \leq m \leq 6$

<table>
<thead>
<tr>
<th>$m$</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>86°</td>
<td>76°</td>
<td>50°</td>
<td>16°</td>
</tr>
</tbody>
</table>

(iii) Instability for $m \geq 6$. 
4.5 Semi-implicit extrapolation methods

4.5.1 Implicit Euler method (h-extrapolation)

\( (*) \quad y_{k+1} = y_k + h f(x_{k+1}, y_{k+1}) \), \( k \geq 0 \), \( y_0 = \alpha \).

\( (*) \) requires the solution of a nonlinear system of equations:

\[
F(y_{k+1}) = y_{k+1} - y_k - h f(x_{k+1}, y_{k+1}).
\]

Newton’s method:

\[
F'(y^{(i)}_{k+1}) = I - h f_y(x_{k+1}, y^{(i)}_{k+1}) =: A_i = \begin{bmatrix}
\frac{\partial f_1}{\partial y_1}(x_{k+1}, y^{(i)}_{k+1}) & \cdots & \frac{\partial f_1}{\partial y_d}(x_{k+1}, y^{(i)}_{k+1}) \\
\vdots & \ddots & \vdots \\
\frac{\partial f_d}{\partial y_1}(x_{k+1}, y^{(i)}_{k+1}) & \cdots & \frac{\partial f_d}{\partial y_d}(x_{k+1}, y^{(i)}_{k+1})
\end{bmatrix}.
\]

Given \( y^{(0)}_{k+1} \), for \( i = 0, 1, 2, \ldots \) compute:

\[
(I - h A_i) \Delta y^{(i)}_{k+1} = - (y^{(i)}_{k+1} - y_k - h f(x_{k+1}, y^{(i)}_{k+1}))
\]

\[
y^{(i+1)}_{k+1} = y^{(i)}_{k+1} + \Delta y^{(i)}_{k+1}.
\]
Idea [Deuflhard (1985)]: Implementation of only one Newton iteration with $y_{k+1}^{(0)} = y_k \implies$

Semi-implicit Euler method:

$$(I - h A) \Delta y_k = -h f(x_{k+1}, y_k),$$

$$y_{k+1} = y_k + \Delta y_k,$$

where $A := f_y(x_{k+1}, y_k)$.

Order and step size control as for the explicit Euler method using the following modification of the sequence for the work units:

$$A_1 = C_J + C_{LR} + n_1 (C_{Subst} + C_f),$$
$$A_i = A_{i-1} + C_J + C_{LR} + n_i C_{Subst} + (n_i - 1) C_f$$

$C_J$ : Evaluation of the Jacobi matrix $A := f_y(x_{k+1}, y_k)$

$C_{LR}$ : LR decomposition of $I - h_i A$

$C_{Subst}$ : Forward and backward substitution in Gauss elimination

$C_f$ : Evaluation of the right-hand side

Code: EULSIM
4.5.2 Semi-implicit midpoint rule ($h^2$-extrapolation) ([Bader/Deuflhard (1983)])

\[ y' - A y = f(x,y) - A y \text{ mit } A := f_y(x,y), \]

\[
\frac{1}{2h} (y_{k+1} - y_k) - \frac{1}{2} A (y_{k+1} + y_k) = f(x_k, y_k) - A y_k.
\]

**Initial step:** Semi-implicit Euler method

\[
(I - h A) \Delta y_0 = h f(y_0),
\]

\[ y_1 = y_0 + \Delta y_0. \]

**Loop:** For $1 \leq k \leq \ell$ compute

\[
(I - h A) y_{k+1} = (I + h A) y_{k-1} + 2 h \left[ f(x_k, y_k) - A y_k \right].
\]

**Bader’s final step:** Instead of $y_{\ell}$ use

\[ \hat{y}_\ell := \frac{1}{2} (y_{\ell+1} + y_{\ell-1}). \]

**Code:** METAN
4.6 Differential-algebraic equations

4.6.1 Linear implicit systems

Definition 4.17 Linear implicit system

Let \( A, B \in \mathbb{R}^{d \times d} \), \( f : I \to \mathbb{R}^d \), \( I := [a, b] \subset \mathbb{R} \), and \( \alpha \in \mathbb{R}^d \). Then,

\[
A \ y'(x) = B \ y(x) + f(x) \quad , \quad x \in I ,
\]

\[
y(a) = \alpha
\]

is called an initial value problem for a linear system of first order ordinary differential equations in implicit form.

We distinguish the following cases:

(i) \( A \) is regular

Reduction to a linear system of first order ordinary differential equations in explicit form

\[
y'(x) = A^{-1} B \ y(x) + A^{-1} f(x) \quad , \quad x \in I .
\]

(ii) \( A \) is singular, \( B \) is regular

Multiplication by \( B^{-1} \) gives

\[
(*) \quad B^{-1} A \ y'(x) = y(x) + B^{-1} f(x) \quad , \quad x \in I .
\]
Let $J$ be the Jordan normal form of the singular matrix $B^{-1}A$, i.e.,

$$B^{-1} A = T \begin{pmatrix} R & 0 \\ 0 & N \end{pmatrix} T^{-1}$$

with a non singular matrix $T \in \mathbb{R}^{d \times d}$, where $R$ corresponds to the non zero eigenvalues of $A$ and $N$ to the eigenvalues $0$ of $A$.

$N$ is nilpotent. Assume that $N$ is nilpotent of index $k \leq d$, i.e., $N^k = 0$.

Using the similarity transformation $T$, the system $(*)$ is transformed to

$$\begin{pmatrix} R & 0 \\ 0 & N \end{pmatrix} T^{-1} y'(x) = T^{-1} y(x) + T^{-1} B^{-1} f(x) .$$

Setting $T^{-1} \alpha = (u \alpha, w \alpha)^T$, we obtain the decoupled system:

$$\begin{align*}
(**)_1 & \quad R \ u'(x) = u(x) + r(x) , \ x \in I , \ u(a) = u \alpha , \\
(**)_2 & \quad N \ w'(x) = w(x) + s(x) , \ x \in I , \ w(a) = w \alpha .
\end{align*}$$
We study the solution of the system

\begin{align*}
(**)_1 & \quad R \ u'(x) = u(x) + r(x), \ x \in I, \ u(a) = u_\alpha, \\
(**)_2 & \quad N \ w'(x) = w(x) + s(x), \ x \in I, \ w(a) = w_\alpha.
\end{align*}

The initial value problem \((**)_1\) has a unique solution. The solution of the initial value problem \((**)_2\) is subject to restrictions:

**Definition 4.18 Index of a matrix**

Let \(C \in \mathbb{R}^{d \times d}\). Then,

\[ k := \min \{ \ell \in \mathbb{N}_0 \mid \text{rank } C^\ell = \text{rank } C^{\ell+1} \} \]

is called the index of the matrix \(C\) and is denoted by \(\text{Ind } C\).

**Lemma 4.19 Nilpotent matrices and index**

If \(N\) is nilpotent of index \(k\), there holds

\[ \text{Ind } (B^{-1} A) = k. \]
We consider the initial value problem

\[(**) \quad N w'(x) = w(x) + s(x), \ x \in I, \ w(a) = w_\alpha.\]

Under the assumption \(s \in C^{k-1}(I)\), by differentiation it follows that

\[
\begin{align*}
w(x) &= -s(x) + N w'(x) \\
w'(x) &= -s'(x) + N w''(x)
\end{align*}
\] \Rightarrow \quad \begin{align*}
w(x) &= -s(x) - N s'(x) + N^2 w''(x) \\
w''(x) &= -s''(x) + N w'''(x)
\end{align*}
\] \Rightarrow \quad \begin{align*}
w(x) &= -s(x) - N s'(x) - N^2 s''(x) + N^3 w'''(x), \\
& \quad \ldots \\
w(x) &= -\sum_{j=0}^{k-1} N^j s^{(j)}(x) + N^k w^{(k)}(x) = 0.
\end{align*}

Hence, we obtain

\[w_a := w(a) = -\sum_{j=0}^{k-1} N^j s^{(j)}(a).\]

**Definition 4.20** Consistency of initial data

The initial data \(\alpha \in \mathbb{R}^d\) is said to be consistent, if \(w_a = -\sum_{j=0}^{k-1} N^j s^{(j)}(a)\).
Remark 4.21 Non differentiable components of the solution

The derivation of the consistency condition does not require the differentiability of all components of $w$. In view of

$\begin{pmatrix}
0 & 1 & 0 & 0 & \cdots & 0 \\
0 & 0 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 1 & \cdots & 0 \\
0 & 0 & 0 & 0 & \cdots & 0
\end{pmatrix}$,

for instance, the first component of $w$ is not effected by the computation of $Nw'$, $N^2w''$ etc. Indeed, it may occur that there are non differentiable components of the solution.
(iii) A and B are arbitrary matrices

Application of regular matrix bundles (cf. [Gantmacher]):

If \( \det (\lambda B - A) \neq 0 \), the linear-implicit system is equivalent to

\[
(\lambda B - A)^{-1} B y' = \begin{bmatrix} (\lambda B - A)^{-1} A y + (\lambda B - A)^{-1} f \end{bmatrix}
\]

Characterization of the solution by Drazin’s inverse \( \hat{B}^D \) of \( \hat{B} \) (cf. [Wilkinson (1982)]).

As in case (ii), a regularity condition on \( f \) and consistency of the initial data are required.
4.6.2 Index of implicit systems of ordinary differential equations

Definition 4.22 Implicit system of first order ordinary differential equations

Assume that $F : D_1 \times D_2 \times I \rightarrow \mathbb{R}^d$, $D_i \subset \mathbb{R}^d$, $I := [a, b] \subset \mathbb{R}$, and $\alpha \in \mathbb{R}^d$. Then,

\[ F(y'(x), y(x), x) = 0 \quad , \quad x \in I \quad , \quad y(a) = \alpha \]

is called an initial value problem for an implicit system of first order ordinary differential equations.

Definition 4.23 Index of an implicit system [Gear (1988)]

Consider the system obtained by differentiation of $(\ast)$:

\[ F(y', y, x) = 0 \quad , \quad \frac{d}{dx} F(y', y, x) = \frac{\partial F}{\partial y'} y'' + \frac{\partial F}{\partial y} y' + \frac{\partial F}{\partial x} = 0 \quad , \quad \quad \cdot \quad , \quad \quad \cdot \quad , \quad \quad \frac{d^\mu}{dx^\mu} F(y', y, x) = \frac{\partial F}{\partial y'} y^{(\mu+1)} + \ldots = 0 . \]

The smallest number $\mu \in \mathbb{N}_0$, for which $(\diamond)$ can be solved for $y'$ explicitly, is called the index of $(\ast)$ and is denoted by $\nu$. 
Definition 4.24  Consistency of the initial data
Assume that \((\ast)\) is of index \(\nu\) Then, the initial data \(y_a\) are called consistent, if
\[
F(y', y, x)|_{y=y(a), x=a} = 0 ,
\]
\[
\cdot = \cdot ,
\]
\[
\frac{d^\nu}{dx^\nu} F(y', y, x)|_{y=y(a), x=a} = 0
\]

Remark 4.25  Special case of linear implicit systems
For linear implicit systems and regular \(A\), we have that \(\nu = \text{Ind}(A^{-1}B)\).

Definition 4.26  Differential-algebraic system
Assume that \(I := [a, b] \subset \mathbb{R}\) and \(D_i \subset \mathbb{R}^d\), \(1 \leq i \leq 3\), as well as
\[
F_1 : D_1 \times D_2 \times D_3 \times I \rightarrow \mathbb{R}^d , \quad F_2 : D_2 \times D_3 \times I \rightarrow \mathbb{R}^d .
\]
Then,
\[
(\ast)_1 \quad F_1(y'(x), y(x), z(x), x) = 0 , \quad x \in I ,
\]
\[
(\ast)_2 \quad F_2(y(x), z(x), x) = 0 , \quad x \in I
\]
is called a semi-implicit system of first order ordinary differential equations in separated form. The characteristic feature is an a priori separation into the differential variable \(y\) and the algebraic variable \(z\). Therefore, it is also referred to as a differential-algebraic system.
Computation of the index of differential-algebraic systems

Idea: Differentiation of the algebraic part $F_2$.

Example 4.27 Systems of index 1

\[
\begin{align*}
(\circ)_1 & \quad y' = f(y, z), \\
(\circ)_2 & \quad 0 = g(y, z).
\end{align*}
\]

Assumption: $\frac{\partial g}{\partial z}$ has a bounded inverse in a neighborhood of the solution.

Differentiation of $(\circ)_2$ yields

\[
0 = \frac{\partial g}{\partial y} y' + \frac{\partial g}{\partial z} z' \implies
\]

\[
z' = -\left(\frac{\partial g}{\partial z}\right)^{-1} \frac{\partial g}{\partial y} y' = -\left(\frac{\partial g}{\partial z}\right)^{-1} \frac{\partial g}{\partial y} f(y, z) \implies
\]

$(\circ)_1, (\circ)_2$ is of index 1. The initial data $(y(a), z(a))^T$ are consistent, if

\[
g(y(a), z(a)) = 0.
\]
Example 4.28 Systems of index 2

\[ \begin{align*}
(\dagger)_1 & \quad y' = f(y, z), \\
(\dagger)_2 & \quad 0 = g(y).
\end{align*} \]

Assumption: \( \frac{\partial g}{\partial y} \frac{\partial f}{\partial z} \) has a bounded inverse in a neighborhood of the solution.

Differentiation of \((\dagger)_2\) results in

\[ (\dagger)_3 \quad 0 = \frac{\partial g}{\partial y} y' = \frac{\partial g}{\partial y} f(y, z) \]

The system \((\dagger)_1, (\dagger)_3\) is of index 1. Consequently, \((\dagger)_1, (\dagger)_2\) is of index 2.

The initial data \((y(a), z(a))^T\) are consistent, if

\[ g(y(a)) = 0, \]

\[ \frac{\partial}{\partial y} (g(y) f(y, z))|_{y=y(a), z=z(a)} = 0. \]
Example 4.29 Systems of index 3

\begin{align*}
\tag{\dagger}_1 & \quad y' = f(y, z), \\
\tag{\dagger}_2 & \quad z' = k(y, z, u), \\
\tag{\dagger}_3 & \quad 0 = g(y).
\end{align*}

Assumption: $\frac{\partial g}{\partial y} \frac{\partial f}{\partial z} \frac{\partial k}{\partial u}$ has a bounded inverse in a neighborhood of the solution.

Differentiating in \(\dagger\)_3 twice, we obtain

\begin{align*}
\tag{\dagger}_4 & \quad 0 = \frac{\partial g}{\partial y} f(y, z), \\
\tag{\dagger}_5 & \quad 0 = \frac{\partial^2 g}{\partial y^2} f(y, z)^T f(y, z) + \frac{\partial g}{\partial y} \left[ \frac{\partial f}{\partial y} f(y, z) + \frac{\partial f}{\partial z} k(y, z, u) \right].
\end{align*}

The system \(\dagger\)_1, \(\dagger\)_2, \(\dagger\)_5 is of index 1. Consequently, \(\dagger\)_1, \(\dagger\)_2, \(\dagger\)_3 is of index 3.

The initial data \((y(a), z(a), u(a))^T\) are consistent, if

\begin{align*}
g(y(a)) &= 0, \\
\frac{\partial g}{\partial y}(y(a), z(a)) &= 0, \\
\frac{\partial^2 g}{\partial y^2} f^T f + \frac{\partial g}{\partial y} \left[ \frac{\partial f}{\partial y} f + \frac{\partial f}{\partial z} k \right]|_{y=y(a), z=z(a), u=u(a)} &= 0.
\end{align*}
4.6.3 Adaptation of stiff integrators

(i) BDF-Verfahren [Gear (1971), Petzold (1981)]

Idea: Replace $y'(x_{j+m})$ by the backward difference quotient

$$D^m y_{j+m} := \frac{1}{h} \sum_{k=0}^{m} \alpha_k y_{j+k}$$

and, given an iterate $y^{(0)}_{j+m}$, solve the nonlinear system

$$F(D^m y_{j+m}, y_{j+m}, x_{j+m}) = 0 \quad 0 \leq j \leq N - m$$

by a Newton or Newton-like method.

Codes: LSODE [Hindmarsh (1980)]
        DASSL [Petzold (1981)]
(ii) Semi-implicit extrapolation methods [Deuflhard/Hairer/Zugck (1987)]

Application of the semi-implicit Euler discretization to quasi-linear ordinary differential equations of index 1

\[(\bullet) \quad B(y) y' = f(y).\]

Construction:

\[
\begin{aligned}
B(y_{k+1}) (y_{k+1} - y_k) &= h f(y_{k+1}) \\
B(y_{k+1}) &= B(y_k) + B_y(y_k) (y_{k+1} - y_k) \\
&\approx h B_y(y) y'_{y(a)} \\
f(y_{k+1}) &= f(y_k) + f_y(y_k) (y_{k+1} - y_k) \\
&\approx f_y(y)_{y(a)}
\end{aligned}
\]

\[
[ B(y_k) - h A ] (y_{k+1} - y_k) = h f(y_k), \quad \text{where} \quad A := \frac{\partial}{\partial y} [ f(y) - B(y) y' ]_{y(a)}.
\]

If \( y'(a) \) is not known:

Set \( A_a := f_y(y(a)) \) and compute \( y'(a) \) later by extrapolation from \( h^{-1}(y_\ell - y_{\ell-1}) \), \( \ell = n_1, n_2, \ldots. \)
Special case: Semi-explicit ordinary differential equation of index 1

\[
\begin{align*}
\circ_1 & \quad y' = f(y, z), \\
\circ_2 & \quad 0 = g(y, z).
\end{align*}
\]

Idea: Application of the semi-implicit Euler discretization to the singularly perturbed system

\[
\begin{align*}
\circ'_1 & \quad y' = f(y, z), \\
\circ'_2 & \quad \varepsilon z' = g(y, z)
\end{align*}
\]

and setting \( \varepsilon = 0 \) afterwards.

Code: LIMEX [Deuflhard/Nowak (1985)]
(iii) Implicit Runge-Kutta methods
We restrict ourselves to 'Fehlberg'-type methods, i.e.,
\[ a_{sj} = b_j , \quad 1 \leq j \leq s . \]

\( \alpha \) Application to semi-explicit systems of index 1:

(i) \[ \begin{cases} Y_i = y(a) + h \sum_{j=1}^{s} a_{ij} f(Y_j, Z_j) , & 1 \leq i \leq s , \\ g(Y_i, Z_i) = 0 , & 1 \leq i \leq s , \end{cases} \]
(ii) \[ y_1 := Y_s , \quad z_1 := Z_s . \]

\( \beta \) Application to quasi-linear systems

(i) \[ Y_i = y(a) + h \sum_{j=1}^{s} a_{ij} U_j , \quad 1 \leq i \leq s , \]
(ii) \[ B(Y_i) U_i = f(Y_i) , \quad 1 \leq i \leq s . \]

Since \( A := (a_{ij})_{i,j=1}^{s} \) is invertible, elimination of \( U_i \) from (ii) by (i). Pay attention to Newton solution of the nonlinear system (ii).

Code: RADAU5 [Hairer/Wanner (1988)]
4.7 Differential-algebraic systems in device simulation

4.7.1 Fundamental electric devices

A linear resistor $R$ between two knots is characterized by a linear relationship between the currents and the voltages according to

$$ R = \frac{U}{I}. $$

For a linear capacity $C$ between two knots we have

$$ C = \frac{Q}{U}, \quad I = \frac{dQ}{dt} = C \frac{dU}{dt}, $$

i.e., there is a linear relationship between the charges and the voltages.

An amplifier amplifies an input signal $U_+ - U_-$ according to

$$ U_{am} = A (U_+ - U_-). $$
4.7.2 Kirchhoff’s laws for electric networks

1. Junction rule

In a junction with a total of $n$ entering resp. leaving currents, the sum of all currents is zero:

$$\sum_{k=1}^{n} I_k = 0 .$$

2. Closed loop rule

Along a closed loop with $m$ elements, the sum of the voltages is zero:

$$\sum_{k=1}^{m} U_m = 0 .$$
4.7.3 Double amplifier

Kirchhoff’s laws in the knots 1 – 4 yield

\[ C_1 (\dot{U}_1 - \dot{U}_{\text{in}}) + \frac{1}{R_1} (U_1 - U_2) = 0 , \]
\[ \frac{1}{R_1} (U_2 - U_1) + C_2 (\dot{U}_2 - \dot{U}_3) - I_1 = 0 , \]
\[ C_2 (\dot{U}_3 - \dot{U}_2) + \frac{1}{R_2} (U_3 - U_4) = 0 , \]
\[ \frac{1}{R_2} (U_4 - U_3) - I_2 = 0 . \]

This has to be completed by the two equations:

\[ U_2 = A (U_1 - U_0) , \]
\[ U_4 = A (U_3 - U_0) . \]
The equations result in the differential-algebraic system:

\[ \dot{C} \dot{X} + B \dot{X} = f, \]

\[ X := (U_1, U_2, U_3, U_4, I_1, I_2)^T, \quad f := (C_1 \dot{U}_{in}, 0, 0, 0, 0)^T, \]

where

\[
C = \begin{pmatrix}
C_1 & 0 & 0 & 0 & 0 & 0 \\
0 & C_2 & -C_2 & 0 & 0 & 0 \\
0 & -C_2 & C_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}, \quad
B = \begin{pmatrix}
\frac{1}{R_1} & -\frac{1}{R_2} & 0 & 0 & 0 & 0 \\
0 & \frac{1}{R_1} & 0 & 0 & -1 & 0 \\
0 & 0 & \frac{1}{R_2} & 0 & 0 & 0 \\
0 & 0 & -\frac{1}{R_2} & \frac{1}{R_2} & 0 & -1 \\
A & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & A & -1 & 0 & 0
\end{pmatrix}.
\]
The differential index is given by \( \text{Ind}(B^{-1}C) \). For \( \hat{C} := B^{-1}C \) we obtain

\[
\hat{C} = \begin{pmatrix}
-\frac{C_1 R_1}{A-1} & 0 & 0 & 0 & 0 & 0 \\
-\frac{C_1 A R_1}{A-1} & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{C_2 R_2}{A-1} - \frac{C_2 R_2}{A-1} & 0 & 0 & 0 & 0 \\
0 & \frac{C_2 A R_2}{A-1} - \frac{C_2 R_2}{A-1} & 0 & 0 & 0 & 0 \\
-C_1 & -C_2 & C_2 & 0 & 0 & 0 \\
0 & C_2 & -C_2 & 0 & 0 & 0
\end{pmatrix}, \quad \hat{C}^2 = \begin{pmatrix}
\left(\frac{C_1 R_1}{A-1}\right)^2 & 0 & 0 & 0 & 0 & 0 \\
\left(\frac{C_1 A R_1}{A-1}\right)^2 A & 0 & 0 & 0 & 0 & 0 \\
-\frac{C_1 C_2 A R_1 R_2}{(A-1)^2} & -\left(\frac{C_2 R_2}{A-1}\right)^2 & \left(\frac{C_2 R_2}{A-1}\right)^2 & 0 & 0 & 0 \\
-\frac{C_1 C_2 A^2 R_1 R_2}{(A-1)^2} & -\left(\frac{C_2 R_2}{A-1}\right)^2 A & \left(\frac{C_2 R_2}{A-1}\right)^2 A & 0 & 0 & 0 \\
\frac{C_2^2 R_1 + C_1 C_2 A R_1}{A-1} & \frac{C_2 R_2}{A-1} C_2 & -\frac{C_2 R_2}{A-1} C_2 & 0 & 0 & 0 \\
-\frac{C_1 C_2 A R_1}{A-1} & -\frac{C_2 R_2}{A-1} C_2 & \frac{C_2 R_2}{A-1} C_2 & 0 & 0 & 0
\end{pmatrix}.
\]

Since \( \text{Ker} \hat{C} = \text{Ker} \hat{C}^2 \), we get \( \text{Ind} \hat{C} = 1 \).