

ETH Lectures 401-0663-00L Numerical Methods for Computer Science
401-2673-00L Numerical Methods for CSE

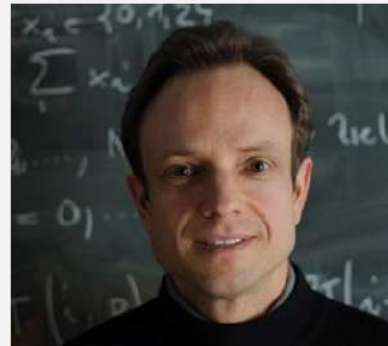
Course Video

Section 12.3: Implicit Runge-Kutta Single-Step Methods

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(C) Seminar für Angewandte Mathematik, ETH Zürich



Tablet notes may have been corrected and/or extended after the recording of the video!

Prerequisites.

- Polynomial interpolation Section 5.2
- Numerical quadrature Chapter 7

Dependencies. Section 11.3.2, Section 11.4 Section 12.1

Duration: minutes

XII. Single-Step Methods for Stiff Initial-Value Problems

12.3 Implicit Runge-Kutta Single-Step Methods

Notion 12.2.0.7. Stiff IVP

An initial value problem is called **stiff**, if stability imposes much tighter timestep constraints on **explicit single step methods** than the accuracy requirements.

12.3.1 The Implicit Euler Method for stiff IVPs

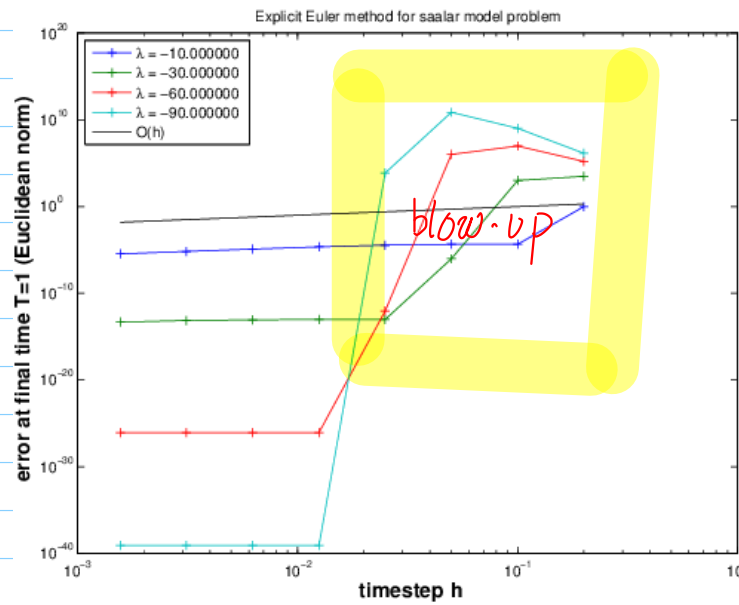
Exp: 12.3.1.1. (Euler methods for stiff decay IVPs)

$$\text{IVP: } \dot{y} = \lambda y, \quad y(0) = 1, \quad \lambda < 0$$

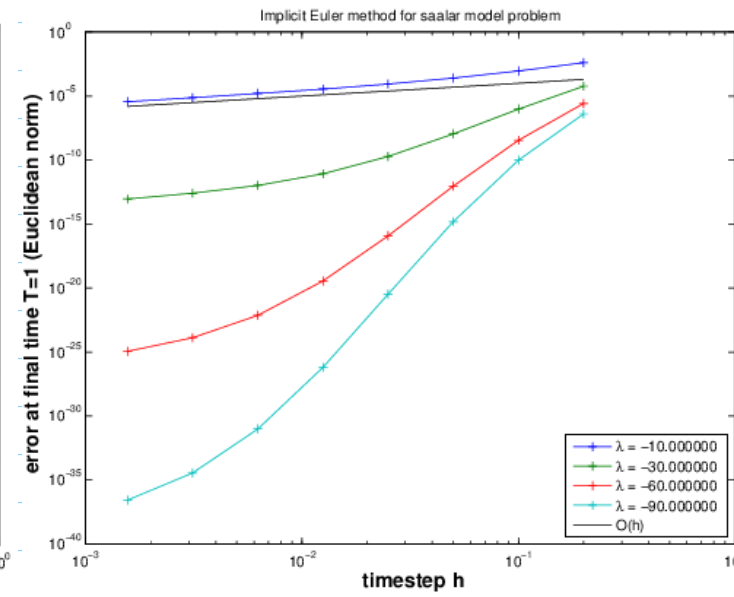
Numerical integrators: The two Euler methods with uniform timestep size $h > 0$

(2)

Explicit Euler method (11.2.1.5)

 λ large: blow-up of y_k for large timestep h

Implicit Euler method (11.2.2.2)

 λ large: stable for all timesteps $h > 0$!

$$N > 1 : \dot{y} = M y, \quad M \in \mathbb{R}^{N,N}$$

$$y(0) = y_0$$

Technique: Diagonalization $\rightarrow$ § 11.1.0.40

Assume: $\exists V \in \mathbb{C}^{N,N} : V^{-1} M V = D = \text{diag}(\lambda_1, \dots, \lambda_N)$

Impl. Euler: $V^{-1} | \quad y_{k+1} = y_k + h M y_{k+1}$

$[z_k := V^{-1} y_k] \quad z_{k+1} = z_k + h \underbrace{V^{-1} M V}_D z_{k+1}$

Decoupling: $(z_{k+1})_l = (z_k)_l + h \lambda_l (z_{k+1})_l, \quad l=1, \dots, N$

$\triangleright (z_k)_l = \left(\frac{1}{1 - h \lambda_l} \right)^k (z_0)_l \xrightarrow{k \rightarrow \infty} 0 \quad \text{if } \text{Re } \lambda_l < 0$

$\forall h > 0$

For any timestep, the implicit Euler method generates exponentially decaying solution sequences $(y_k)_{k=0}^\infty$ for $\dot{y} = M y$ with diagonalizable matrix $M \in \mathbb{R}^{N,N}$ with eigenvalues $\lambda_1, \dots, \lambda_N$, if $\text{Re } \lambda_i < 0$ for all $i = 1, \dots, N$.

Unconditional stability: no timestep constraint!

§ 12.3.1.2 (Linear model problem analysis of implicit Euler method) $\rightarrow$ § 11.1.0.41

Linear model problem: $\dot{y} = \lambda y, \quad y(0) = y_0, \quad \text{Re } \lambda < 0$

[solution $y(t) = e^{\lambda t} \rightarrow 0$ for $t \rightarrow \infty$]

Impl. Euler recursion: $y_{k+1} : y_{k+1} = y_k + h \lambda y_{k+1}$

$\Leftrightarrow y_{k+1} = \frac{1}{1 - h \lambda} y_k$

$\triangleright y_k = \left(\frac{1}{1 - h \lambda} \right)^k y_0 \xrightarrow{k \rightarrow \infty} 0 \quad \forall h > 0$

③ 12.3.2 Collocation Single-Step Methods

Goal: Unconditionally stable SSMs of higher order

ODE: $\dot{y} = f(t, y)$, $f: I \times D \rightarrow \mathbb{R}^N$

§ 12.3.2.1. (Collocation approach)

(Focus on 1st step: $y_0 \rightarrow y_1$, time interval $[t_0, t_1]$)

- $t \rightarrow y_n(t) \triangleq$ approximation of solution $y(t)$

$$y_n \in V \subset (C^1([t_0, t_1]))^N, \dim V = N(s+1)$$

$\hookrightarrow \triangleq$ trial space with $s \leq N$ fixed

- $N(s+1)$ Collocation conditions:

$$y_n|_{t_0} = y_0$$

$$\dot{y}_n(\tau_j) = f(\tau_j, y_n(\tau_j)) : \text{pointwise satisfaction of ODE}$$

$$\text{for } t_0 \leq \tau_1 < \tau_2 < \dots < \tau_s \leq t_1$$

$\triangleq$ collocation points

$$y_1 := y_n(t_1) = y_0 + h \sum_{j=1}^s k_j \int_0^1 L_j(\varphi) d\varphi$$

§ 12.3.2.4 (Polynomial collocation)

"Standard choice": $V = (\mathcal{P}_s)^N$

$$\tau_j := t_0 + c_j h, \quad h := t_1 - t_0, \quad 0 \leq c_1 < c_2 < \dots < c_s \leq 1$$

Recall: **II** Lagrange polynomials L_j

- $L_j \in \mathcal{P}_{s-1}$, $j = 1, \dots, s$

- $L_j(c_\ell) = \delta_{j\ell}$ [$\rightarrow$ cardinal basis]

$$y_n \in V \Rightarrow \dot{y}_n \in (\mathcal{P}_{s-1})^N$$

$$\Rightarrow \dot{y}_n(t_0 + \bar{j}h) = \sum_{j=1}^s \dot{y}_n(t_0 + c_j h) L_j(\bar{j}), \quad 0 \leq \bar{j} \leq 1$$

$$\xrightarrow{\text{ODE}} = \sum_{j=1}^s \underbrace{f(t_0 + c_j h, y_n(t_0 + c_j h))}_{=: k_j \in \mathbb{R}^N} L_j(\bar{j})$$

Integrate $[y_0|_{t_0} = y_0]$

$$y_n(t_0 + \bar{j}h) = y_0 + h \sum_{j=1}^s k_j \int_0^{\bar{j}} L_j(\varphi) d\varphi$$

$$\triangleright k_i = f(t_0 + c_i h, y_0 + h \sum_{j=1}^s k_j \int_0^{c_j} L_j(\varphi) d\varphi), \quad 1 \leq i \leq s \quad (*)$$

4 Rem. 12.3.2.7 (Implicit collocation SSM)

(*) $\leftrightarrow$ N -s non-linear equations for $k_1, \dots, k_s \in \mathbb{R}^N$
 ("implicit")

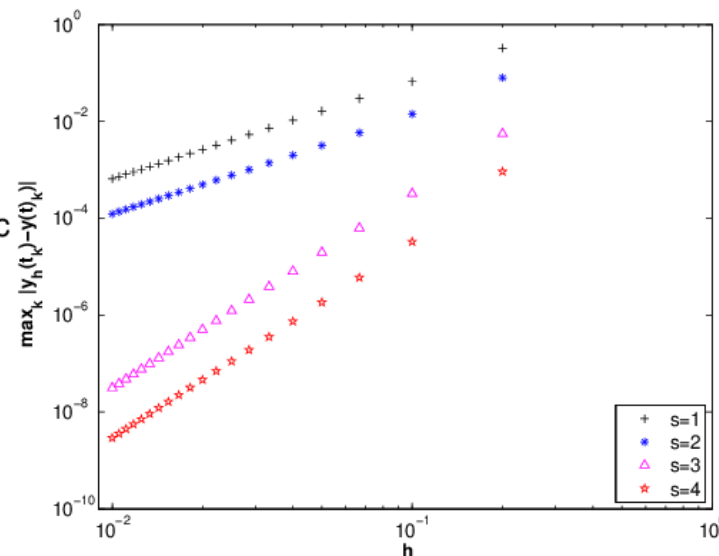
Exp. 12.3.2.10. (Convergence of collocation SSMs)

- IVP: $\dot{y} = \lambda y(1-y)$, $y(0) = 0.01$, $\lambda = 100$
- Collocation SSM on $[0,1]$ w/ uniform timestep $h > 0$

1 Equidistant collocation points, $c_j = \frac{j}{s+1}$,
 $j = 1, \dots, s$.

We observe algebraic convergence with the empiric rates

$s = 1$	: $p = 1.96$
$s = 2$	: $p = 2.03$
$s = 3$	: $p = 4.00$
$s = 4$	: $p = 4.04$



$\triangleright$ Rate $\begin{cases} s, & \text{even } s \\ s+1, & \text{odd } s \end{cases} \leftrightarrow$ order of coll. SSM



Implicit Euler = coll SSM!

§ 12.3.2.8 (Collocation SSM and quadrature)

$$\left. \begin{array}{l} \dot{y} = f(t) \\ y(0) = 0 \end{array} \right\} \Rightarrow y_1 = h \sum_{j=1}^s f(t_0 + c_j h) \int_0^1 L_j(\vartheta) d\vartheta$$

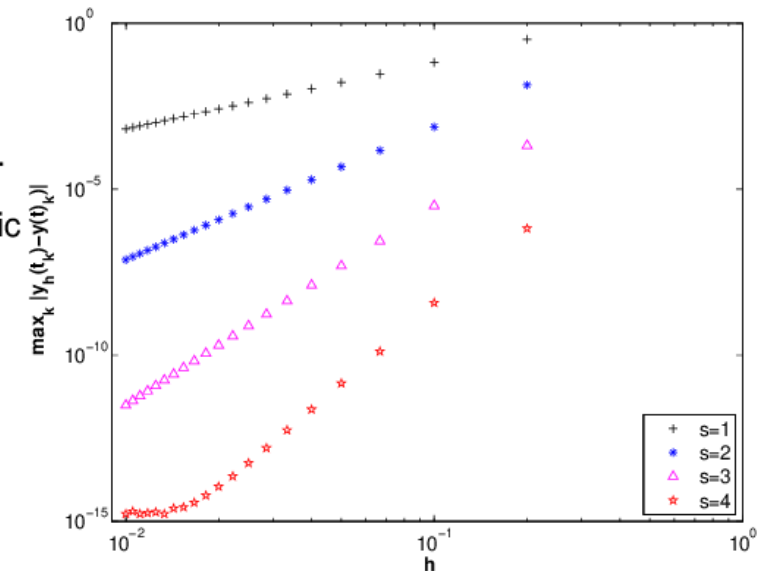
$\hat{=}$ s -pt. quadrature formula on $[0,1]$ with nodes c_j

Exp. 12.3.2.10 cont'd :

1 Gauss points in $[0,1]$
 as normalized collocation points c_j , $j = 1, \dots, s$.

We observe algebraic convergence with the empiric rates

$s = 1$	: $p = 1.96$
$s = 2$	: $p = 4.01$
$s = 3$	: $p = 6.00$
$s = 4$	: $p = 8.02$



$\triangleright$ Order = $2s$!

Theorem 12.3.2.12. Order of collocation single step method

Provided that $\mathbf{f} \in C^p(I \times D)$, the order ($\rightarrow$ Def. 11.3.2.8) of an s -stage collocation single step method according to (12.3.2.6) agrees with the order ($\rightarrow$ Def. 7.4.1.1) of the quadrature formula on $[0, 1]$ with nodes c_j and weights b_j , $j = 1, \dots, s$.

12.3.3 General Implicit RK-SSMs

Summary: Collocation SSM for $\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y})$

$$\mathbf{k}_i = \mathbf{f}(t_0 + c_i h, \mathbf{y}_0 + h \sum_{j=1}^s a_{ij} \mathbf{k}_j), \quad \text{where} \quad a_{ij} := \int_0^{c_i} L_j(\tau) d\tau, \quad (12.3.2.6)$$

$$\mathbf{y}_1 := \mathbf{y}_h(t_1) = \mathbf{y}_0 + h \sum_{i=1}^s b_i \mathbf{k}_i.$$

$$b_i := \int_0^1 L_i(\tau) d\tau.$$

Compare:

Definition 11.4.0.11. Explicit Runge-Kutta single-step method

For $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{i-1} a_{ij}$, $i, j = 1, \dots, s$, $s \in \mathbb{N}$, an s -stage explicit Runge-Kutta single step method (RK-SSM) for the ODE $\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y})$, $\mathbf{f} : \Omega \rightarrow \mathbb{R}^N$, is defined by ($\mathbf{y}_0 \in D$)

$$\mathbf{k}_i := \mathbf{f}(t_0 + c_i h, \mathbf{y}_0 + h \sum_{j=1}^{i-1} a_{ij} \mathbf{k}_j), \quad i = 1, \dots, s, \quad \mathbf{y}_1 := \mathbf{y}_0 + h \sum_{i=1}^s b_i \mathbf{k}_i.$$

The vectors $\mathbf{k}_i \in \mathbb{R}^N$, $i = 1, \dots, s$, are called **increments**, $h > 0$ is the size of the timestep.

Definition 12.3.3.1. General Runge-Kutta single step method (cf. Def. 11.4.0.11)

For $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^s a_{ij}$, $i, j = 1, \dots, s$, $s \in \mathbb{N}$, a single step of size $h > 0$ of an s -stage **Runge-Kutta single step method** (RK-SSM) for the IVP (11.1.3.2) is defined by

$$\mathbf{k}_i := \mathbf{f}(t_0 + c_i h, \mathbf{y}_0 + h \sum_{j=1}^s a_{ij} \mathbf{k}_j), \quad i = 1, \dots, s, \quad \mathbf{y}_1 := \mathbf{y}_0 + h \sum_{i=1}^s b_i \mathbf{k}_i.$$

As before, the vectors $\mathbf{k}_i \in \mathbb{R}^N$ are called **increments**.

$N_s \times N_s$ non-linear system of equations

Notation:

General Butcher scheme notation for RK-SSM

Shorthand notation for Runge-Kutta methods

Butcher scheme

$\triangleright$

$$\begin{array}{c|c} \mathbf{c} & \mathcal{A} \\ \hline & \mathbf{b}^T \end{array} := \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}. \quad (12.3.3.3)$$

Note that now, in contrast to (11.4.0.13), $\mathcal{A}$ can be a general $s \times s$ -matrix.

⑥

Rem 12.3.3.6 (Stage-form equations for increments)

(for autonomous ODE $\dot{y} = \underline{f}(y)$)

$$\underset{\substack{\uparrow \text{ stages}}}{g_i} := h \sum_{j=1}^s a_{ij} k_j \iff \underset{\substack{\uparrow \text{ increments}}}{k_i} = \underline{f}(y_0 + g_i)$$

▷ Stage equations:

$$k_i = \underline{f}\left(y_0 + h \sum_{j=1}^s a_{ij} k_j\right)$$

$$\iff g_i = h \sum_{j=1}^s a_{ij} \underline{f}(y_0 + g_j)$$

$$\Rightarrow y_1 = y_0 + h \sum_{i=1}^s b_i \underline{f}(y_0 + g_i)$$

Note: $|h| \ll 1 \Rightarrow g_i \approx 0$

▷ Zero is a good initial guess for stages!

Rem 12.3.3.9 (Solving the stage equations)

$$g_i = h \sum_{j=1}^s a_{ij} \underline{f}(y_0 + g_j) \iff \vec{g} = \begin{bmatrix} g_1 \\ \vdots \\ g_s \end{bmatrix} \in \mathbb{R}^{N \cdot s}$$

$$F(\vec{g}) = \vec{g} - h \left(\underset{\substack{\uparrow \text{ Kronecker product } \in \mathbb{R}^{N_s, N_s}}}{A \otimes I_N} \right) \begin{bmatrix} \underline{f}(y_0 + g_1) \\ \vdots \\ \underline{f}(y_0 + g_s) \end{bmatrix} = 0$$

Apply simplified Newton method w/ $\vec{g}^{(0)} = \underline{0}$ ■

$$\vec{g}^{(m+1)} = \vec{g}^{(m)} - DF(0)^{-1} \vec{g}^{(m)}, m = 0, 1, 2, \dots$$

$$DF(0) = I_{N_s} - h A \otimes D\underline{f}(y_0) \in \mathbb{R}^{N_s, N_s}$$

$$\downarrow \\ = I_{N_s} \text{ for } h = 0 \Rightarrow \text{invertible for small } |h|$$

7

12.3.4 Model Problem Analysis for IRK-SSMs

Scalar linear ODE : $\dot{y} = \lambda y$, $\lambda \in \mathbb{C}$
 $\downarrow$ RK-SSM
 $y_{k+1} = S(h\lambda) y_k$

Theorem 12.3.4.4. Stability function of Runge-Kutta methods, cf. Thm. 12.1.0.17

The discrete evolution Ψ_λ^h of an s -stage Runge-Kutta single step method ($\rightarrow$ Def. 12.3.3.1) with Butcher scheme $\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array}$ (see (12.3.3.3)) for the ODE $\dot{y} = \lambda y$ is given by a multiplication with

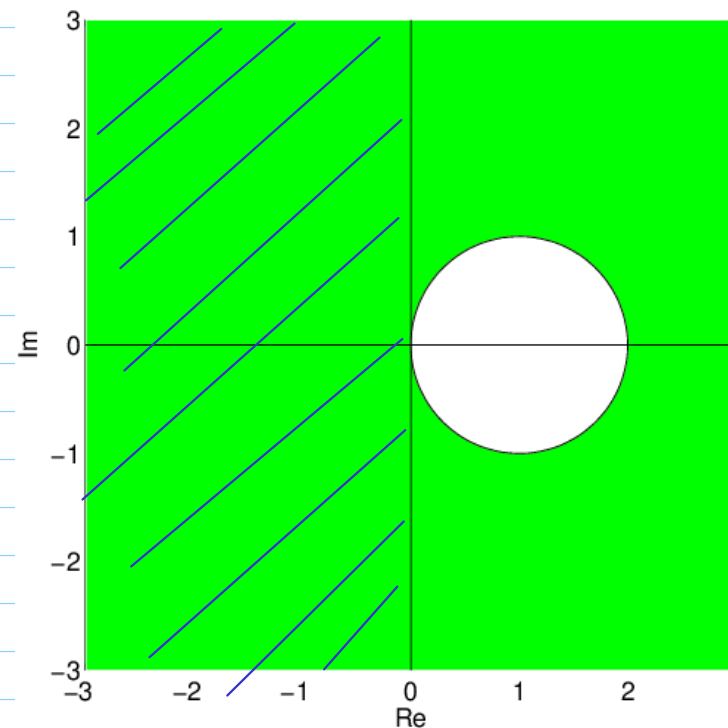
$$S(z) := \underbrace{1 + z\mathbf{b}^T(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{1}}_{\text{stability function}} = \frac{\det(\mathbf{I} - z\mathbf{A} + z\mathbf{1}\mathbf{b}^T)}{\det(\mathbf{I} - z\mathbf{A})}, \quad z := \lambda h, \quad \mathbf{1} = [1, \dots, 1]^T \in \mathbb{R}^s.$$

Cramer's rule

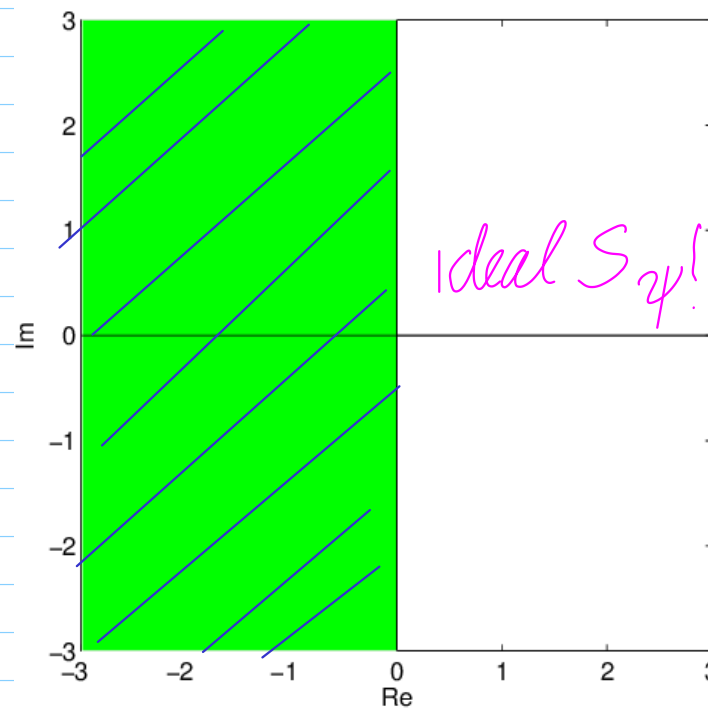
$\rightarrow$ A rational function
 $S(z) = \frac{p(z)}{q(z)}, p, q \in \mathcal{P}_s$

Region of stability

$$S_\Psi := \{z \in \mathbb{C} : |S(z)| < 1\}$$



S_Ψ : implicit Euler method (11.2.2.2)



S_Ψ : implicit midpoint method (11.2.3.3)

Ex. 12.3.4.5 (Stability functions of simple IRK-SSMs)

Implicit Euler method:

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

$\rightarrow$

$$S(z) = \frac{1}{1-z}$$

Implicit midpoint method:

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

$\rightarrow$

$$S(z) = \frac{1 + \frac{1}{2}z}{1 - \frac{1}{2}z}$$

• S_Ψ unbounded

• $\operatorname{Re} \lambda < 0 \Rightarrow h\lambda \in S_\Psi \quad \forall h > 0$

$\hat{=}$ unconditional stability

§ 12.3.4.7 (A-stability)

Definition 12.3.4.9. A-stability of a Runge-Kutta single step method

A Runge-Kutta single step method with stability function S is **A-stable**, if

$$\mathbb{C}^- := \{z \in \mathbb{C} : \operatorname{Re} z < 0\} \subset \mathcal{S}_\Psi. \quad (\mathcal{S}_\Psi \triangleq \text{region of stability Def. 12.1.0.51})$$

A-stable Runge-Kutta single step methods will not be affected by stability induced timestep constraints when applied to **stiff** IVP ($\rightarrow$ Notion 9.2.7.16). $\rightarrow$ *unconditionally stable*

§ 12.3.4.10 ("Ideal" region of stability*)

Remember: $S(z) \approx \exp(z)$

$$* \mathcal{S}_\Psi^* := \{z \in \mathbb{C} : |\exp(z)| < 1\} = \mathbb{C}^-$$

$$\text{II} \quad |\exp(x+iy)| = e^x \Leftrightarrow x < 0 :$$

For $\dot{y} = \lambda y$:

$$\operatorname{Re} \lambda < 0 \Rightarrow \begin{cases} (y_k) \xrightarrow{k \rightarrow \infty} 0 \\ y(t) \xrightarrow{t \rightarrow \infty} 0 \end{cases}$$

$$\operatorname{Re} \lambda > 0 \Rightarrow \begin{cases} (y_k) \xrightarrow{k \rightarrow \infty} \infty \\ y(t) \xrightarrow{t \rightarrow \infty} \infty \end{cases}$$

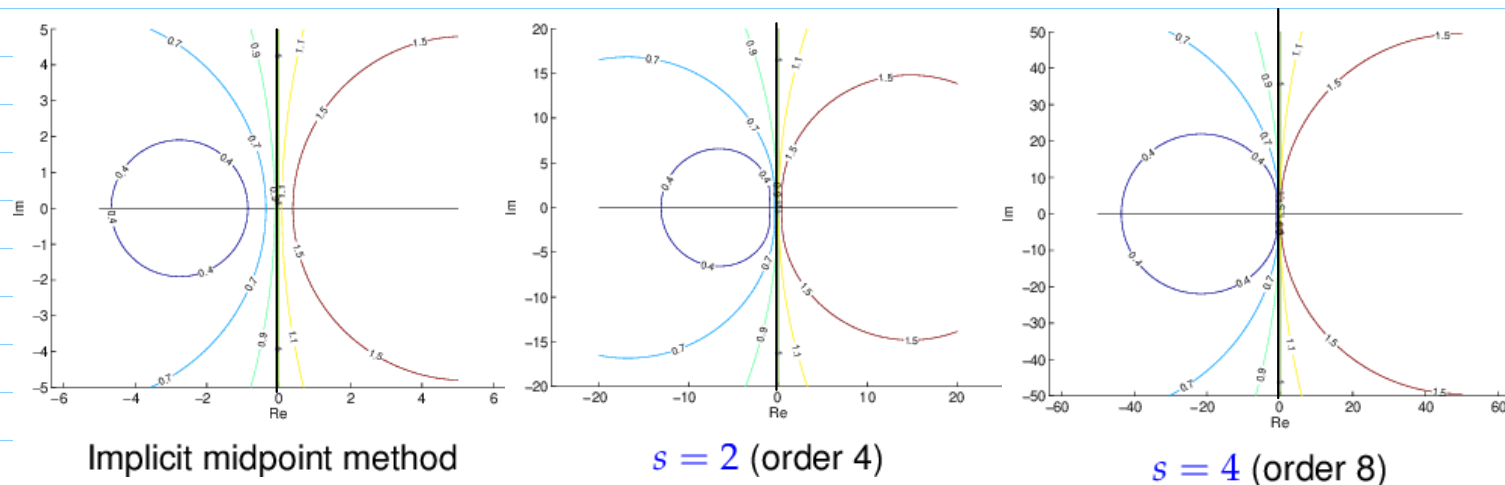
$$\mathcal{S}_\Psi = \mathbb{C}^- \Rightarrow$$

$$[y_{k+1} = S(h\lambda)y_k]$$

RK-SSMs with $\mathcal{S}_\Psi = \mathbb{C}^-$?
 $\rightarrow$ implicit midpoint method

Implicit midpoint method: $\frac{1}{2} \mid \frac{1}{2}$ $\rightarrow$ $S(z) = \frac{1 + \frac{1}{2}z}{1 - \frac{1}{2}z}$

Level lines of $|S(z)|$ for Gauss collocation SSMs:



Theorem 12.3.4.12. Region of stability of Gauss collocation single step methods

s -stage **Gauss collocation single step methods** defined by (12.3.2.6) with the nodes c_s given by the s Gauss points on $[0, 1]$, feature the "ideal" stability domain:

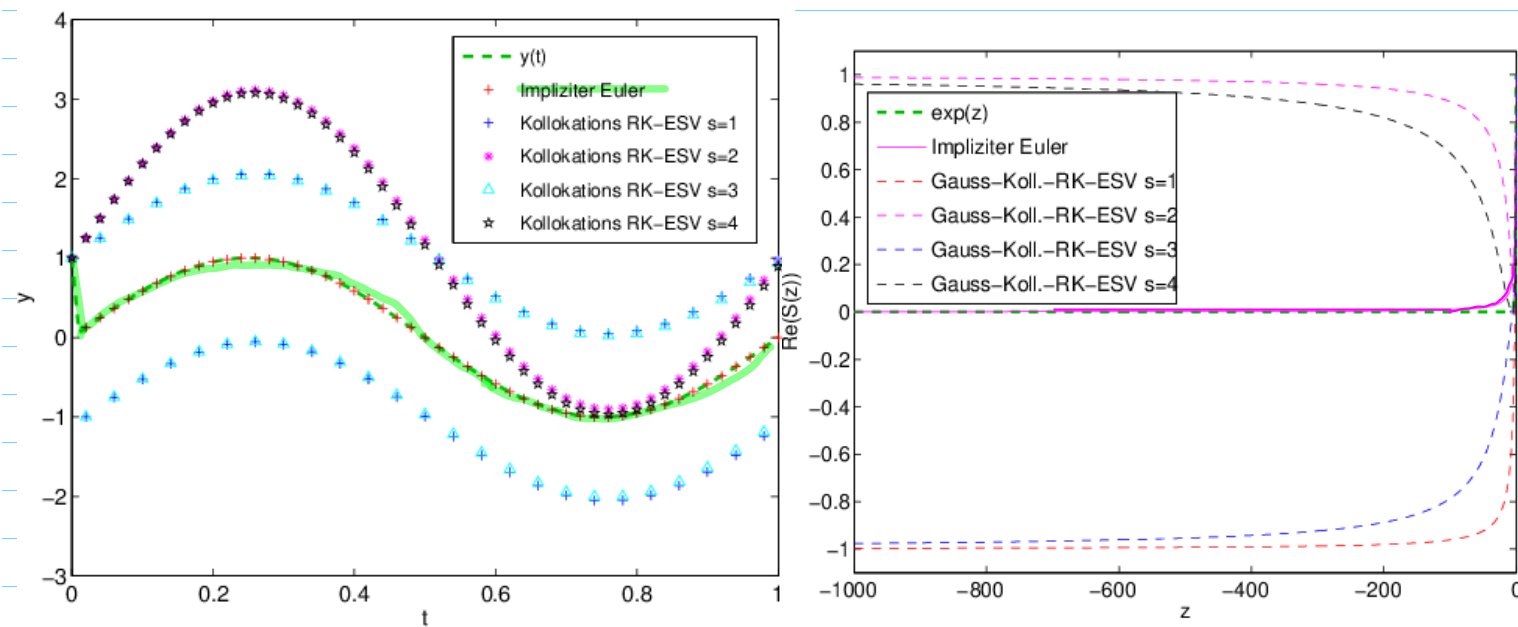
$$\mathcal{S}_\Psi = \mathbb{C}^- . \quad (12.3.4.11)$$

In particular, all Gauss collocation single step methods are A-stable.

9 Exp. 12.3.4.13 (RK-SSMs for stiff IVP)

IVP: $\dot{y} = -\lambda y + \beta \sin(2\pi t)$, $\lambda = 10^6$, $\beta = 10^6$, $y(0) = 1$,

$\triangleright y(t) \approx \sin(2\pi t)$ after very short time



Solutions by RK-SSMs

Stability functions on $\mathbb{R}^-$

For Gauss coll. SSMs

hardly any damping $\triangleleft |S(z)| \rightarrow 1$ as $z \rightarrow -\infty$

vs. $e^z \rightarrow 0$ as $z \rightarrow -\infty$

Impl. Euler: $S(z) = \frac{1}{1-z} \rightarrow 0$ for $z \rightarrow -\infty$

§ 12.3.4.14 (L-stability)

Definition 12.3.4.15. L-stable Runge-Kutta method $\rightarrow$

A Runge-Kutta method ($\rightarrow$ Def. 12.3.3.1) is **L-stable/asymptotically stable**, if its stability function ($\rightarrow$ Thm. 12.3.4.4) satisfies

$$(i) \quad \text{Re } z < 0 \Rightarrow |S(z)| < 1, \quad (12.3.4.16)$$

$$(ii) \quad \lim_{\text{Re } z \rightarrow -\infty} S(z) = 0. \quad (12.3.4.17)$$

L-stable $\iff$ A-stable & " $S(-\infty) = 0$ "

Rem 12.3.4.18 (Necessary condition for L-stability of RK-SSM)

RK-SSM with Butcher scheme $\begin{array}{c|c} A & \\ \hline & b^T \end{array}$

Thm 12.3.4.4

$\triangleright$ Stability function $S(z) = 1 + z \underline{b}^T (I - zA)^{-1} \underline{1} = 1 + \underline{b}^T (\frac{1}{z} I - A)^{-1} \underline{1}$

$\triangleright S(-\infty) = 1 - \underline{b}^T A^{-1} \underline{1} \stackrel{!}{=} 0$

$\triangleright$ If $\underbrace{(A)_{*1}}_{\underline{b}^T A^{-1} = \underline{e}_x^T} = \underline{b} \Rightarrow "S(-\infty) = 0"$

(16)

Butcher scheme (12.3.3.3) for L-stable RK-methods, see Def. 12.3.4.15

$$\triangleright \begin{array}{c|c} \mathbf{c} & \mathbf{a} \\ \hline \mathbf{b}^T & \end{array} := \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_{s-1} & a_{s-1,1} & \cdots & a_{s-1,s} \\ 1 & b_1 & \cdots & b_s \end{array}$$

Ex. 12.3.4.21 (L-stable IRK-SSMs)

s-stage Gauss-Radau methods (collocation SSMs)

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

Implicit Euler method

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

Radau RK-SSM, order 3

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

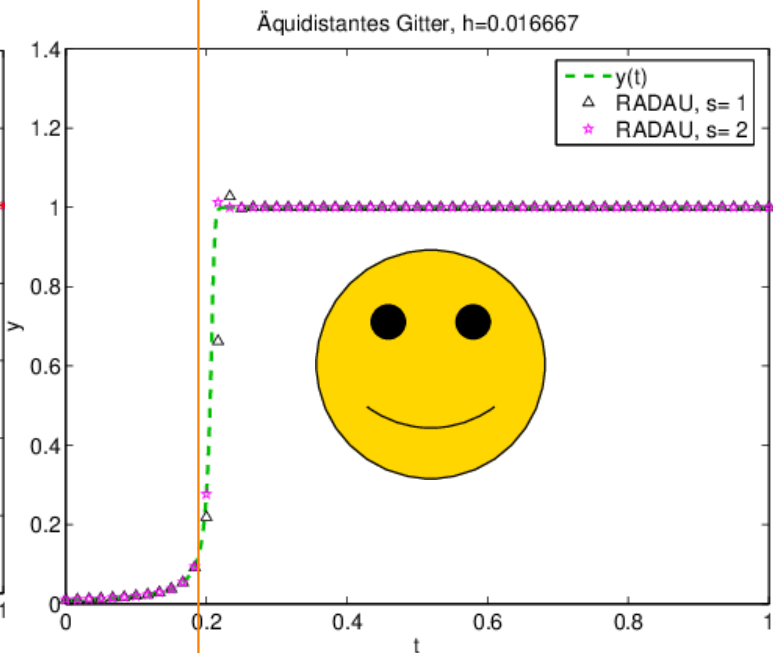
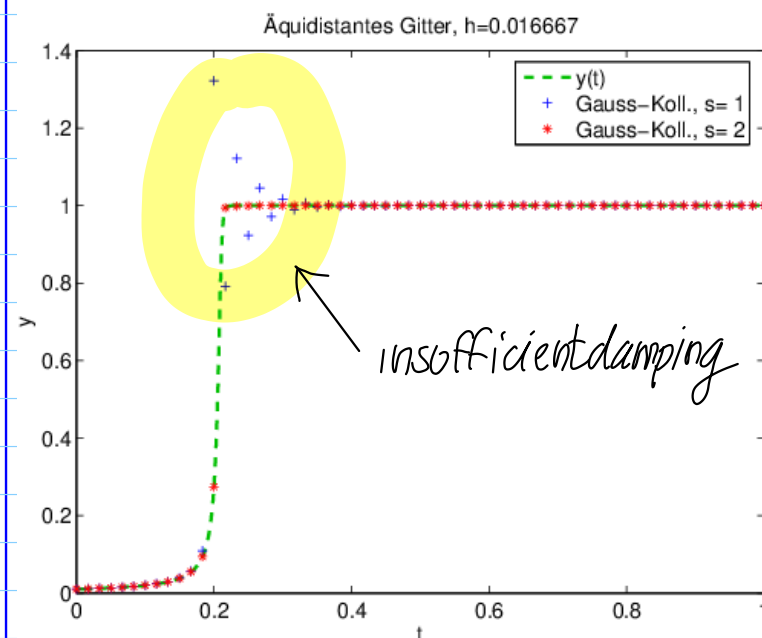
Radau RK-SSM, order 5

$$\text{Order} = 2s - 1$$

Exp. 12.3.4.22 (Gauss-Radau SSMs for stiff IVP)

$$\text{IVP: } \dot{y}(t) = \lambda y^2(1-y), \quad \lambda = 500, \quad y(0) = \frac{1}{100}$$

- Uniform timesteps on $[0, 1]$



All L-stable

