ETH Lecture 401-0663-00L Numerical Methods for CSE

Numerical Methods for Computational Science and Engineering

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URL: http://www.sam.math.ethz.ch/~hiptmair/tmp/NumCSE/NumCSE16.pdf

XII. Single-Step Methods for Stiff IVPs

MATLAB-script 12.0.2: Use of MATLAB integrator ode45 for a stiff problem

```
fun = @(t,x) 500*x^2*(1-x);
options = odeset('reltol',0.1,'abstol',0.001,'stats','on');
[t,y] = ode45(fun,[0 1],y0,options);
```

order used for stepsize control

The option `stats = 'on'` makes MATLAB print statistics about the run of the integrators.

```
186 successful steps
55 failed attempts
1447 function evaluations
```

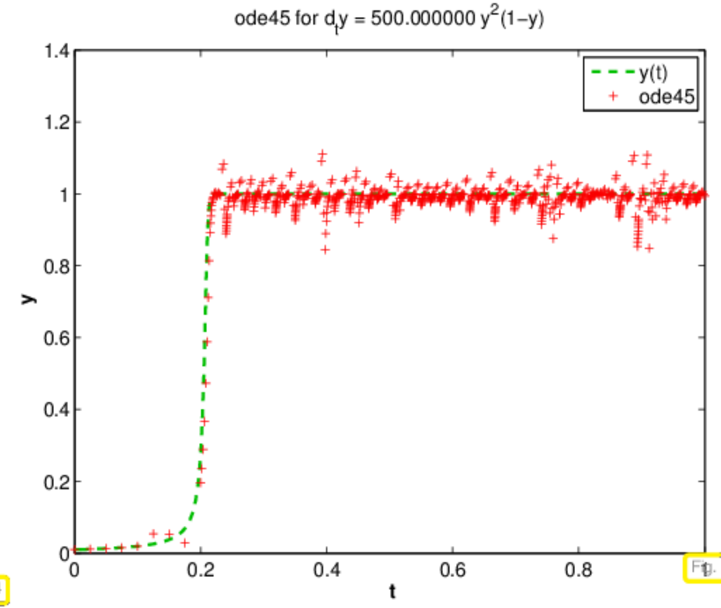


Fig. 424

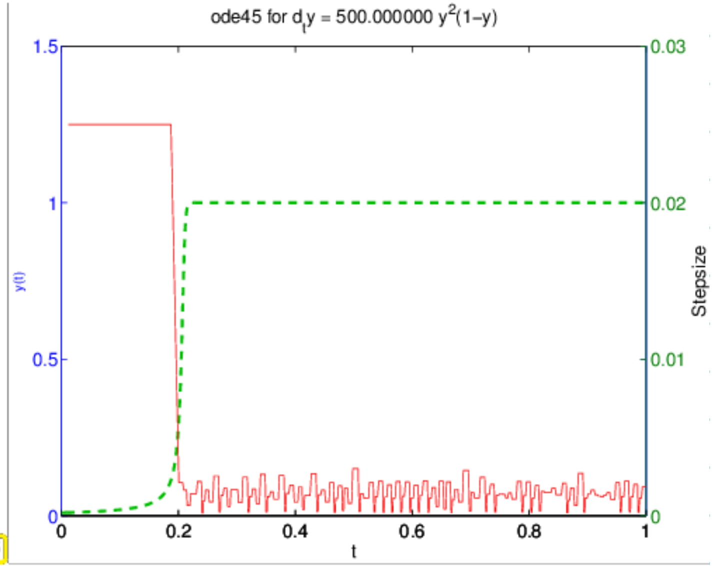


Fig. 425

12.1 Model Problem Analysis

Explicit Euler for $\dot{y} = \lambda y$, $y(0) = 1$

$y(t) = e^{\lambda t} \to 0$ for $t \to \infty$ ↳ decay equation, $\lambda < 0$

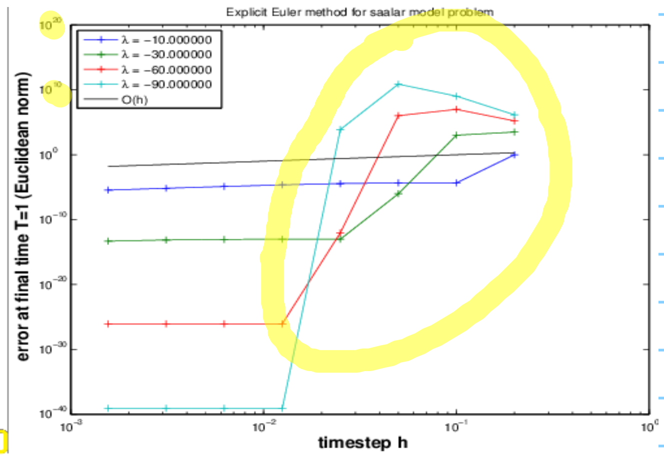


Fig. 426

→ blow-up of y_k for big h

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

Expl. Euler: for $f(y)=\lambda y$ $\quad y_{k+1} = y_k + \lambda h y_k = (1+\lambda h) y_k$

$$\triangleright \quad y_k = (1+\lambda h)^k y_0$$

If $|1+\lambda h| > 1 \Rightarrow y_k \to \pm\infty$ for $k\to\infty$

$ < 1 \Rightarrow y_k \to 0$

$|\lambda h| > 2 \Rightarrow$ blow-up

$\hookrightarrow \quad h < \frac{2}{|\lambda|}$: timestep constraint

Ex.: Expl. trapezoidal method

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac12 & \frac12 \end{array} \quad \Rightarrow \quad \begin{aligned} k_1 &= f(y_0) \\ k_2 &= f(y_0 + h k_1) \\ y_1 &= y_0 + \tfrac12 h (k_0 + k_1) \end{aligned}$$

$$\dot y = \lambda y: \quad y_1 = \underbrace{(1+\lambda h + \tfrac12 (\lambda h)^2)}_{=: S(\lambda h)} y_0$$

$$y_k = S(\lambda h)^k y_0$$

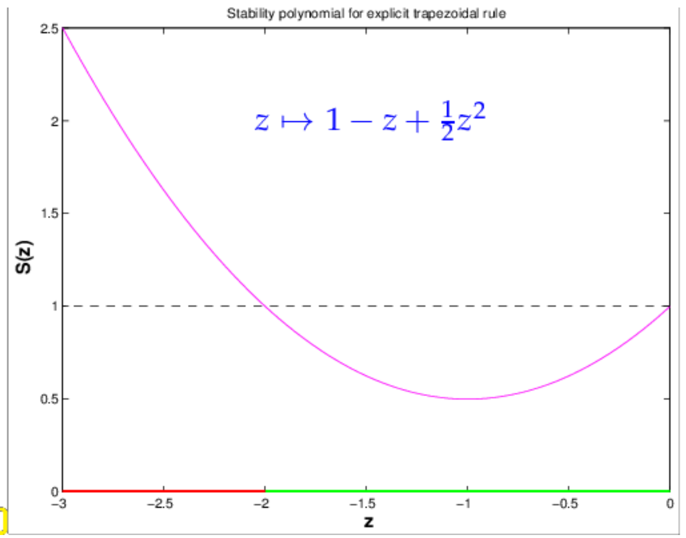


Fig. 432

Clearly, blow-up can be avoided only if $|S(h\lambda)| \le 1$:

$$|S(h\lambda)| < 1 \quad \Leftrightarrow \quad -2 < h\lambda < 0\,.$$

Qualitatively correct decay behavior of $(y_k)_k$ only under timestep constraint

$$h \le |2/\lambda|\,. \qquad (12.1.10)$$

◁ the stability function for the explicit trapezoidal method

Definition 11.4.9. Explicit Runge-Kutta 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 $\dot{\mathbf{y}} = \mathbf{f}(t,\mathbf{y})$, $\mathbf{f}:\Omega\to\mathbb{R}^d$, is defined by ($\mathbf{y}_0 \in D$)

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

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

for $f(y) = \lambda y$: $\quad \in \mathbb{R}^{s,s}$ from Butcher scheme $\quad z := \lambda h$

$$\blacktriangleright \quad \begin{aligned} k_i &= \lambda(y_0 + h\sum_{j=1}^{i-1} a_{ij} k_j)\,, \\ y_1 &= y_0 + h\sum_{i=1}^{s} b_i k_i \end{aligned} \quad \Rightarrow \quad \begin{bmatrix} \mathbf{I} - z\mathfrak{A} & 0 \\ -z\mathbf{b}^\top & 1 \end{bmatrix} \begin{bmatrix} \mathbf{k} \\ y_1 \end{bmatrix} = y_0 \begin{bmatrix} \mathbf{1} \\ 1 \end{bmatrix}, \qquad (12.1.12)$$

$$y_1 = (1 + z\underline{b}^T (I - z\mathcal{A})^{-1} \mathbb{1})\, y_0$$

Theorem 12.1.15. Stability function of explicit Runge-Kutta methods → [?, Thm. 77.2], [?, Sect. 11.8.4]

The discrete evolution Ψ^h_λ *of an explicit* s*-stage Runge-Kutta single step method (→ Def. 11.4.9) with Butcher scheme* $\begin{array}{c|c}\mathbf{c} & \mathfrak{A}\\ \hline & \mathbf{b}^T\end{array}$ *(see (11.4.11)) for the ODE* $\dot{y} = \lambda y$ *amounts to a multiplication with the number*

$$\Psi^h_\lambda = S(\lambda h) \quad \Leftrightarrow \quad y_1 = S(\lambda h) y_0 \,,$$

where S *is the stability function*

$$S(z) := 1 + z\mathbf{b}^T(\mathbf{I} - z\mathfrak{A})^{-1}\mathbf{1} = \det(\mathbf{I} - z\mathfrak{A} + z\mathbf{1}\mathbf{b}^T) \,, \quad \mathbf{1} := [1,\dots,1]^\top \in \mathbb{R}^s \,. \qquad (12.1.16)$$

$$\Rightarrow \quad y_k = S(\lambda h)^k y_0$$

$$|S(\lambda h)| > 1 \quad \Rightarrow \quad \text{blow-up for } k \to \infty$$

Explicit Euler method (11.2.7): $\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$ ➤ $S(z) = 1 + z \,.$

Explicit trapezoidal method (11.4.6): $\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$ ➤ $S(z) = 1 + z + \frac{1}{2}z^2 \,.$

Classical RK4 method: $\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6} \end{array}$ ➤ $S(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4 \,.$

Corollary 12.1.18. Polynomial stability function of explicit RK-SSM

For a consistent (→ Def. 11.3.10) s*-stage explicit Runge-Kutta single step method according to Def. 11.4.9 the stability function* S *defined by (12.1.16) is a non-constant polynomial of degree* $\leq s$*:* $S \in \mathcal{P}_s$.

$$\Rightarrow \quad \lim_{z \to \infty} |S(z)| = \infty$$

$$\mathcal{S}_\Psi := \{ z : |S(z)| \leq 1 \} \quad \text{is bounded}$$

$z = \lambda h$

$\Rightarrow$

$\Rightarrow$ timestep constraint necessary to avoid blow-up

Only if one ensures that $|\lambda h|$ is sufficiently small, one can avoid exponentially increasing approximations y_k (qualitatively wrong for $\lambda < 0$) when applying an explicit RK-SSM to the model problem (12.1.3) with uniform timestep $h > 0$,

Next simplest model problem: Linear system of ODE

$$\dot{y} = My \,, \quad M \in \mathbb{R}^{d,d}$$

Consider circuit from Ex. 11.1.13 ▷

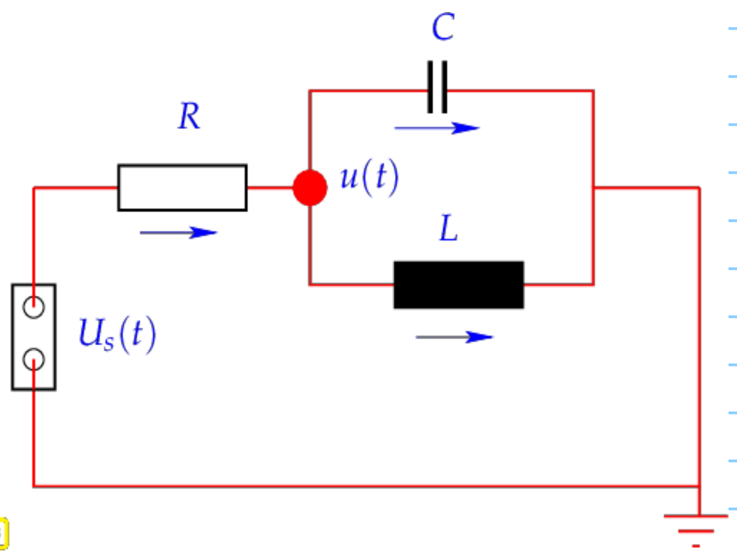


Fig. 433

Transient nodal analysis leads to the second-order linear ODE

$$\ddot u + \alpha \dot u + \beta u = g(t)\,,$$

with coefficients $\alpha := (RC)^{-1}$, $\beta = (LC)^{-1}$, $g(t) = \alpha \dot U_s(t)$.

$$\Downarrow$$

$$\underbrace{\begin{bmatrix}\dot u\\ \dot v\end{bmatrix}}_{=:\dot{\mathbf y}} = \underbrace{\overset{\mathbf M}{\begin{bmatrix}0&1\\-\beta&-\alpha\end{bmatrix}}\begin{bmatrix}u\\v\end{bmatrix} - \begin{bmatrix}0\\g(t)\end{bmatrix}}_{=:\mathbf f(t,\mathbf y)}\,.$$

$\beta \gg \alpha \gg 1$

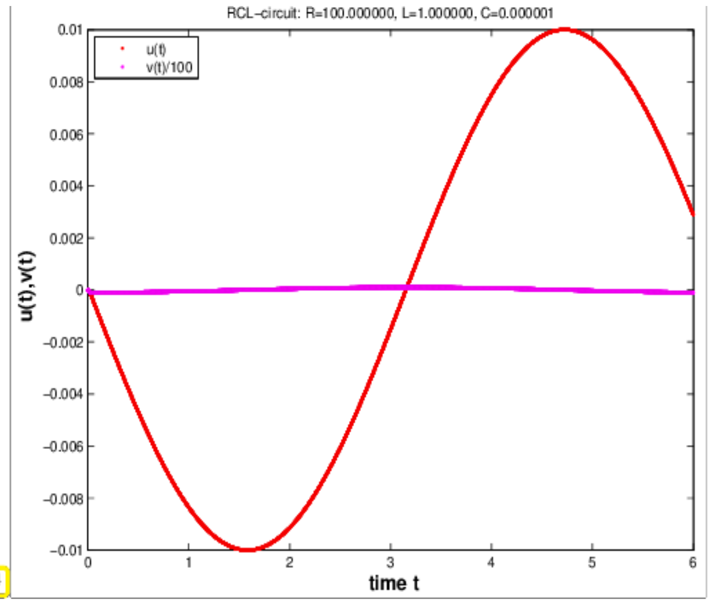


Fig. 434

$R = 100\Omega$, $L = 1\mathrm{H}$, $C = 1\mu\mathrm{F}$, $U_s(t) = 1\mathrm{V}\sin(t)$, $u(0) = v(0) = 0$ ("switch on")

ode45 statistics:
```
17897 successful steps
1090 failed attempts
113923 function evaluations
```

Inefficient: way more timesteps than required for resolving smooth solution, *cf.* remark in the end of § 12.1.24.

Expl. Euler: $\dot{\mathbf y} = \mathbf M \mathbf y$

Diagonalize: $\mathbf V^{-1}\mathbf M\mathbf V = \mathbf D = \mathrm{diag}(\lambda_1,\dots,\lambda_d) \in \mathbb C^{d,d}$

eigenvalue

▷ Sol. of ODE: $\mathbf y(t) = \mathbf V\,\mathrm{diag}(e^{\lambda_i t})_{i=1}^{d}\,\mathbf V^{-1}\mathbf y_0$

If $\mathrm{Re}\,\lambda_i < 0 \Rightarrow \mathbf y(t) \to 0$ for $t \to \infty$

E.E.: $\mathbf y_{k+1} = \mathbf y_k + h\mathbf M\mathbf y_k = \mathbf y_k + h\mathbf V\mathbf D\mathbf V^{-1}\mathbf y_k$

$\mathbf z_k := \mathbf V^{-1}\mathbf y_k \Rightarrow \mathbf z_{k+1} = \mathbf z_k + h\mathbf D\mathbf z_k$

(*) $\underbrace{(\mathbf z_{k+1})_i = (\mathbf z_k)_i + h\lambda_i(\mathbf z_k)_i}_{\text{E. Eul. recursion for } \dot z = \lambda_i z}$

Blow-up of $\mathbf y_k \iff \|\mathbf z_k\| \to \infty$ for $k \to \infty$

$\iff |(\mathbf z_k)_i| \to \infty$ for $k \to \infty$ and one $i \in \{1,\dots,d\}$

$\overset{(*)}{\iff} |1 + h\lambda_i| > 1$ for some $i \in \{1,\dots,d\}$

⑤ Avoid blow-up : $h < \frac{2}{|\lambda_i|} \quad \forall i = 1,\dots,d$

Repetition : Model problem : $\dot{y} = \lambda y$, $\lambda < 0$

RK-SSM (s-stage) : $y_{k+1} = S(\lambda h) y_k$

$\uparrow$ Stability function $\in \mathcal{P}_s$

no blow-up of (y_k) $\Longleftrightarrow$ $\underbrace{|S(\lambda h)| \leq 1}$

$\rightarrow$ timestep constraint

Definition 11.4.9. Explicit Runge-Kutta 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 $\dot{\mathbf{y}} = \mathbf{f}(t,\mathbf{y})$, $\mathbf{f} : \Omega \to \mathbb{R}^d$, is defined by ($\mathbf{y}_0 \in D$)

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

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

Apply to $\dot{y} = My = VDV^{-1}y$

$$k_i = M\left(y_0 + h\sum_{j=1}^{i-1} a_{ij} k_j\right) \quad \Big|\cdot V^{-1}$$

$z_k = V^{-1} y_k$, $k = 0,1$

$\hat{k}_i := V^{-1} k_i$

$\Rightarrow$ $\hat{k}_i = D\left(z_0 + h \sum_{j=1}^{i-1} a_{ij} \hat{k}_j\right)$ $\leftarrow$ decoupled

$z_1 = z_0 + h \sum_{i=1}^{s} b_i \hat{k}_i$

$\Rightarrow$ $\left[\; (\hat{k}_i)_\ell = \lambda_\ell \left((z_0)_\ell + h \sum_{j=1}^{i-1} a_{ij} (\hat{k}_j)_\ell \right) \right]$, $\ell = 1,\dots,d$

$$\begin{array}{ccc}
\dot{y} = My & \xrightarrow{\text{Diagonalization}} & \dot{z}_\ell = \lambda_\ell z_\ell, \; \ell = 1,\dots,d \\
\downarrow \text{RK-SSM} & & \downarrow \text{RK-SSM} \\
\Psi_h & \xrightarrow{\text{Diagonalization}} & \Psi_{\ell,h} \\
[\, y_1 = \Psi_h y_0 \,] & & [\text{RK-SSM disc evol. for } \dot{z}_\ell = \lambda_\ell z_\ell \,]
\end{array}$$

No blow-up of (y_k) $\Longleftrightarrow$ no blow-up for $(z_{\ell,k})_k$

Theorem 12.1.46. (Absolute) stability of explicit RK-SSM for linear systems of ODEs

The sequence $(\mathbf{y}_k)_k$ of approximations generated by an explicit RK-SSM (→ Def. 11.4.9) with stability function S (defined in (12.1.16)) applied to the linear autonomous ODE $\dot{\mathbf{y}} = \mathbf{M}\mathbf{y}$, $\mathbf{M} \in \mathbb{C}^{d,d}$, with uniform timestep $h > 0$ decays exponentially for every initial state $\mathbf{y}_0 \in \mathbb{C}^d$, if and only if $|S(\lambda_i h)| < 1$ for all eigenvalues λ_i of $\mathbf{M}$.

Recall : Even if $M \in \mathbb{R}^{d,d}$: $\lambda_i \in \mathbb{C}$ possible

$\rightarrow$ Study $|S(z)|$ also for $z \in \mathbb{C}$

Definition 12.1.49. Region of (absolute) stability

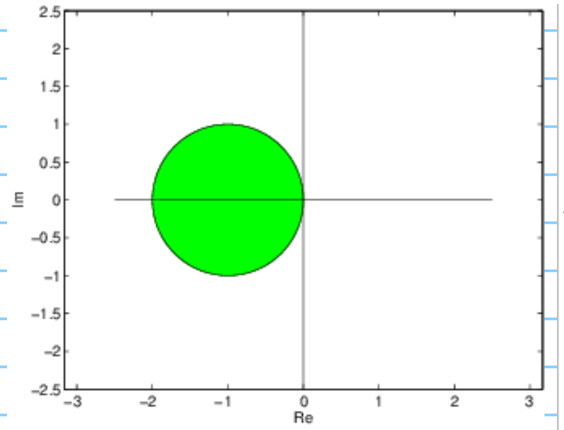
Let the discrete evolution $\mathbf{\Psi}$ for a single step method applied to the scalar linear ODE $\dot{y} = \lambda y$, $\lambda \in \mathbb{C}$, be of the form

$$\mathbf{\Psi}^h y = S(z)y\,, \quad y \in \mathbb{C}, h > 0 \quad \text{with} \quad z := h\lambda \tag{12.1.50}$$

and a function $S : \mathbb{C} \to \mathbb{C}$. Then the region of (absolute) stability of the single step method is given by

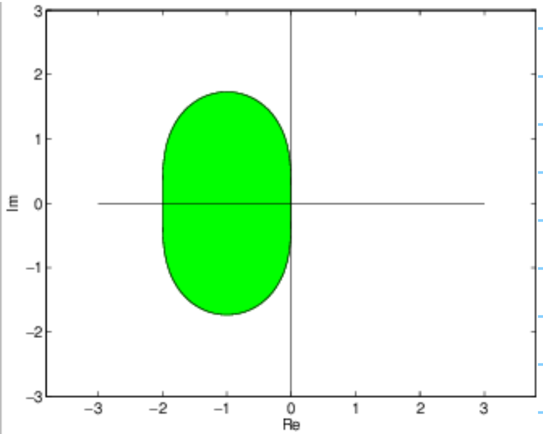
$$\mathcal{S}_{\mathbf{\Psi}} := \{z \in \mathbb{C}: |S(z)| < 1\} \subset \mathbb{C}\,.$$

$y_k = S(z)^k y_0 \Rightarrow |y_k| = |S(z)|^k |y_0|$

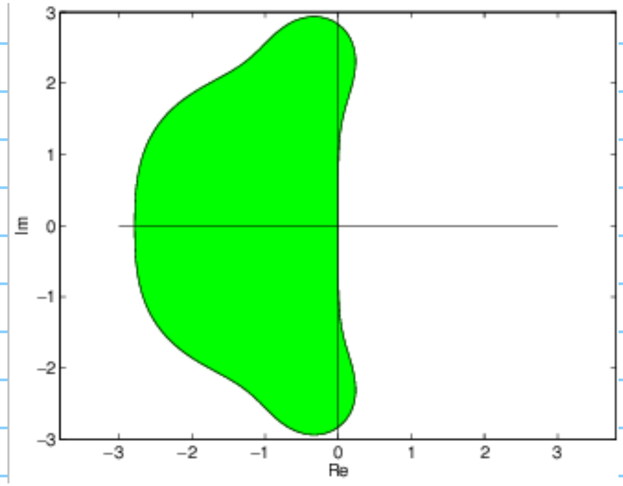


$\mathcal{S}_{\mathbf{\Psi}}$: explicit Euler (11.2.7)

$S(z) = 1 + z$



$\mathcal{S}_{\mathbf{\Psi}}$: explicit trapezoidal method



$\mathcal{S}_{\mathbf{\Psi}}$: classical RK4 method

12.2. Stiff initial value Problems

Ex: $\dot{\mathbf{y}} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \mathbf{y} + \lambda(1 - \|\mathbf{y}\|^2)\mathbf{y}$

If $\|\mathbf{y}_0\| = 1 \Rightarrow \|\mathbf{y}(t)\| = 1$

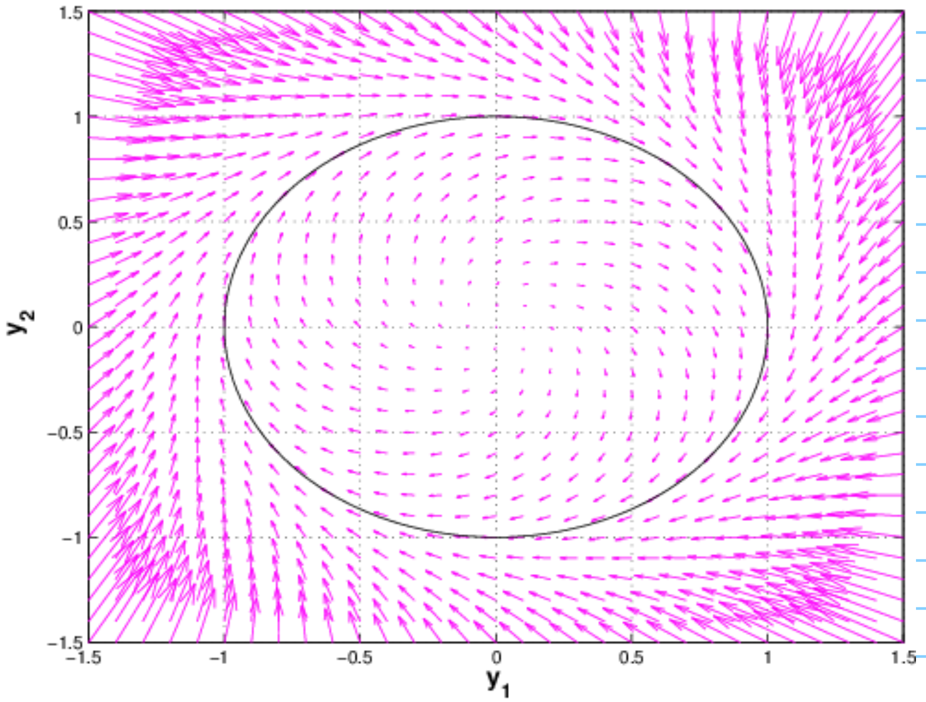


Fig. 439

vectorfield $\mathbf{f}$ ($\lambda = 1$)

$\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$

for $t \ll 1$: $\mathbf{y}(t) \approx \mathbf{y}_0$

Linearize: $\underbrace{\dot{\mathbf{y}} \underset{=}{\approx} \mathbf{f}(\mathbf{y}_0) + D\mathbf{f}(\mathbf{y}_0)(\mathbf{y} - \mathbf{y}_0)}_{\text{(affine) linear ODE}}$

$[\ \dot{\mathbf{y}} = \mathbf{M}\mathbf{y} + \mathbf{b}\ ]$

$\Rightarrow$ For small times $t \to \mathbf{y}(t)$ behaves like the solution of an affine linear ODE

"Linearization of RK-SSM"

$$\begin{array}{ccc} \dot{\mathbf{y}} = \mathbf{f}(\mathbf{y}) & \xrightarrow{\text{Linearization}} & \dot{\mathbf{y}} = D\mathbf{f}(\mathbf{y}_0)\mathbf{y} + \mathbf{b} \\ \text{RK-SSM} \downarrow & & \downarrow \text{RK-SSM} \\ \Psi_h & \xrightarrow[\text{of increment equ. (by Taylor exp.)}]{\text{Linearization}} & \tilde{\Psi}_h \end{array}$$

for small timestep the behavior of an explicit RK-SSM applied to $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$ close to the state $\mathbf{y}_0$ is determined by the eigenvalues of the Jacobian $\mathrm{D}\,\mathbf{f}(\mathbf{y}_0)$.

If $Df(y_0)$ has an eigenvalue λ with large modulus $\Rightarrow$ time-step constraint to avoid blow-up

[However, if $\mathrm{Re}\,\lambda > 0$ $\Rightarrow$ $y(t)$ grows exponentially $\to$ blow-up of numerical solution not a concern.]

Ex cnt'd:

$$\dot{\mathbf{y}} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}\mathbf{y} + \lambda(1 - \|\mathbf{y}\|^2)\,\mathbf{y}\;, \quad \|\mathbf{y}_0\|_2 = 1\;. \quad , \lambda \gg 1 \tag{12.2.6}$$

satisfies $\|\mathbf{y}(t)\|_2 = 1$ for all times. Using the product rule (8.4.10) of multi-dimensional differential calculus, we find

$$\mathrm{D}\,\mathbf{f}(\mathbf{y}) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} + \lambda\left(-2\mathbf{y}\mathbf{y}^\top + (1 - \|\mathbf{y}\|_2^2\mathbf{I})\right)\;.$$

► $\sigma(\mathrm{D}\,\mathbf{f}(\mathbf{y})) = \left\{-\lambda - \sqrt{\lambda^2 - 1}, -\lambda + \sqrt{\lambda^2 - 1}\right\}$, if $\|\mathbf{y}\|_2 = 1$.

[EV $\hat{=}$ eigenvalue] $\quad$ Re EV $\ll 0$ $\quad$ Re EV ≈ 0

$\hookrightarrow$ expect a severe timestep constraint to achieve $|S(\mathrm{EV}\cdot h)| \leq 1$

Example: $\dot{y} = f(y) = \lambda y^2(1-y)$, $\lambda \gg 1$

$y = 1$: $f'(1) = -\lambda$

$\to$ Behavior of adaptive RK-SSM

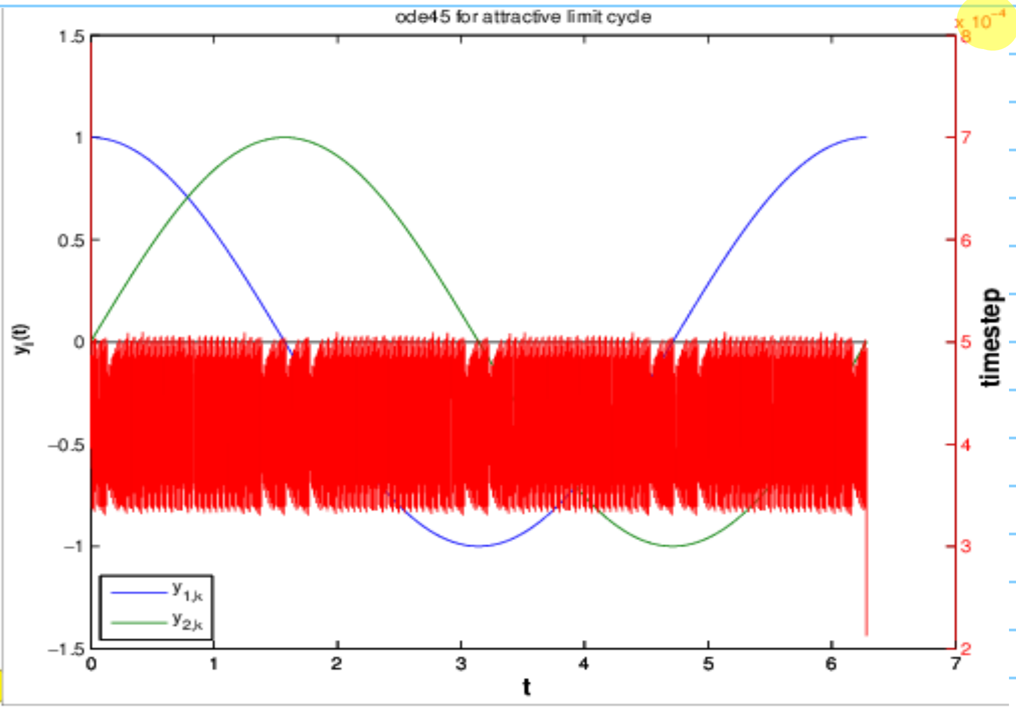


Fig. 441

many (3794) steps ($\lambda = 1000$)

$\to$ tiny timesteps $\downarrow$ in order to avoid blow-up

▷ Stability induced timestep constraint

9

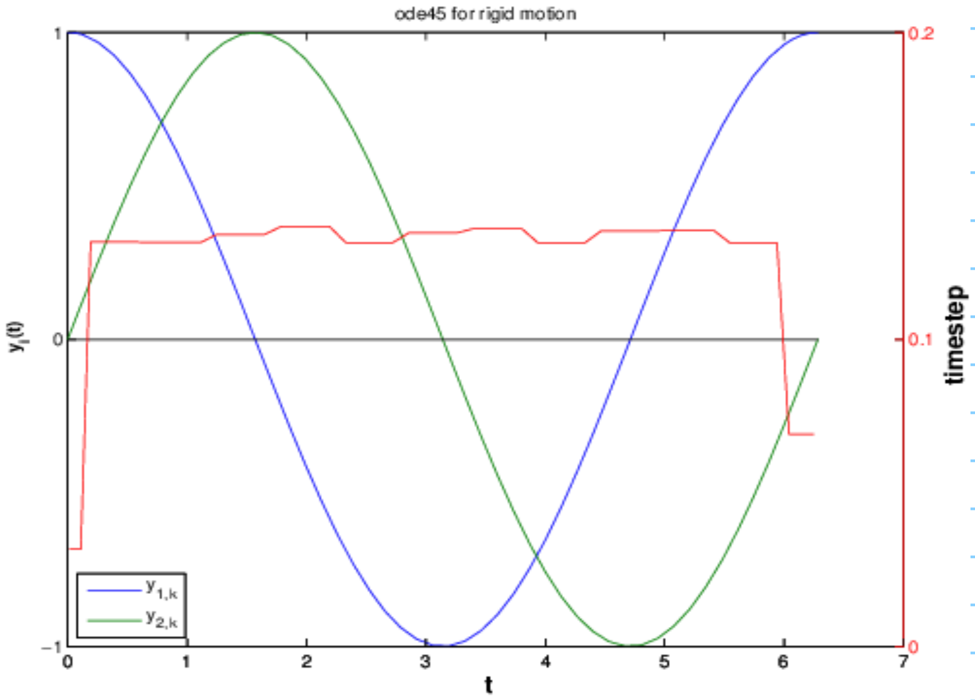


Fig. 442

→ good resolution with large timesteps

accurate solution with few steps ($\lambda = 0$)

Notion 12.2.9. 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.

How to distinguish stiff initial value problems

An initial value problem for an autonomous ODE $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$ will probably be stiff, if, for substantial periods of time,

$$\min\{\operatorname{Re}\lambda : \lambda \in \sigma(\mathrm{D}\,\mathbf{f}(\mathbf{y}(t)))\} \ll 0\,, \qquad (12.2.15)$$

$$\max\{0, \operatorname{Re}\lambda : \lambda \in \sigma(\mathrm{D}\,\mathbf{f}(\mathbf{y}(t)))\} \approx 0\,, \qquad (12.2.16)$$

where $t \mapsto \mathbf{y}(t)$ is the solution trajectory and $\sigma(\mathbf{M})$ is the spectrum of the matrix $\mathbf{M}$, see Def. 9.1.1.

Typical features of stiff IVPs:
- Presence of fast transients in the solution, see Ex. 12.1.1, Ex. 12.1.33,
- Occurrence of strongly attractive fixed points/limit cycles, see Ex. 12.2.5

12.3. Implicit RK-SSM

12.3.1. Implicit Euler method for stiff IVPs

$$\dot{y} = \lambda y\,, \quad \lambda \ll 0$$

1. Eul. [timestep h] : $\quad y_{k+1} = y_k + h\lambda y_{k+1}$

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

no blow-up $\Leftrightarrow$ $\left|\frac{1}{1-h\lambda}\right| \leq 1$: satisfied $\forall h \geq 0$!

→ unconditional stability

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

▷ Impl. Euler immune to stability induced timestep constraints for stiff IVP

☹ only 1-st order

☹ implicit

Higher-order generalizations of impl. Euler :

Definition 12.3.18. General Runge-Kutta single step method (*cf.* Def. 11.4.9)

For $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{s} a_{ij}$, $i,j = 1,\dots,s$, $s \in \mathbb{N}$, an s-stage Runge-Kutta single step method (RK-SSM) for the IVP (11.1.20) is defined by

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

non-linear system of equ. with $s \cdot d$ unknowns

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

Impl. Euler: $s = 1$, $a_{11} = 1$, $b_1 = 1$

General Butcher scheme notation for RK-SSM

Shorthand notation for Runge-Kutta methods

Butcher scheme

Note: now $\mathfrak{A}$ can be a general $s \times s$-matrix.

$$\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array} := \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \;. \tag{12.3.20}$$

▷ Coefficients by solving so-called order equations

↳ tabulated

→ Increment equation are usually solved by simplified Newton method :

$$x^{(k+1)} = x^{(k)} - DF(x^{(0)})^{-1} F(x^{(k)})$$

for $F(x) = 0$

Stage form of increment equations for $\dot{y} = f(y)$

$d=1$: $g_i := h\sum_{j=1}^{s} a_{ij} k_j \Leftrightarrow k_i = f(y_0 + g_i)$

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

$$\vec{g} := \begin{bmatrix} g_1 \\ \vdots \\ g_s \end{bmatrix} : \quad \Updownarrow \quad F(\vec{g}) = 0$$

with $F(\vec{g}) := \vec{g} - h\mathfrak{A} \begin{bmatrix} f(y_0+g_1) \\ \vdots \\ f(y_0+g_s) \end{bmatrix}$

Initial guess : $\vec{g}^{(0)} = \underline{0}$

$$DF(\underline{0}) = I - h\mathfrak{A} \begin{bmatrix} f'(y_0) & & \\ & \ddots & \\ & & f'(y_0) \end{bmatrix} \in \mathbb{R}^{s,s}$$

12.3.4 Model problem analysis for implicit RK-SSM

Apply RK-SSM : $\dot{y} = \lambda y$ [$\rightarrow$ linear ODE]

Definition 12.3.18. General Runge-Kutta single step method (*cf.* Def. 11.4.9)

For $b_i, a_{ij} \in \mathbb{R}$, $c_i := \sum_{j=1}^{s} a_{ij}$, $i, j = 1, \dots, s$, $s \in \mathbb{N}$, an s-stage Runge-Kutta single step method (RK-SSM) for the IVP (11.1.20) is defined by

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

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

$$k_i = \lambda (y_0 + h \sum_{j=1}^{s} a_{ij} k_j) \qquad z := \lambda h$$

$$y_1 = y_0 + h \sum b_i k_i$$

$$\Leftrightarrow \begin{bmatrix} I - z\mathfrak{A} & 0 \\ -h\underline{b}^T & 1 \end{bmatrix} \begin{bmatrix} k_1 \\ \vdots \\ k_s \\ y_1 \end{bmatrix} = \begin{bmatrix} \lambda y_0 \\ \vdots \\ \lambda y_0 \\ y_0 \end{bmatrix}$$

$$\Rightarrow \quad y_1 = y_0 + h \underline{b}^T (I - z\mathfrak{A})^{-1} \lambda y_0 \mathbb{1} = S(z) y_0$$

Theorem 12.3.27. Stability function of Runge-Kutta methods, *cf.* Thm. 12.1.15

[Stability function of general Runge-Kutta methods]
The discrete evolution Ψ^h_λ of an s-stage Runge-Kutta single step method ($\rightarrow$ Def. 12.3.18) with Butcher scheme $\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array}$ (see (12.3.20)) for the ODE $\dot{y} = \lambda y$ is given by a multiplication with

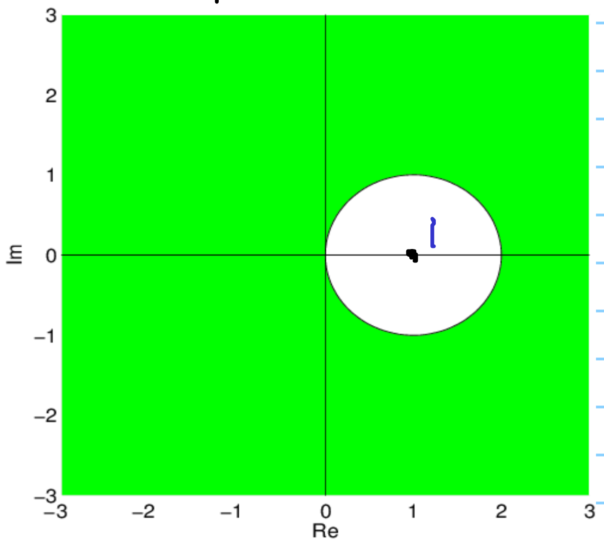
$$S(z) := \underbrace{1 + z\mathbf{b}^T(\mathbf{I} - z\mathfrak{A})^{-1}\mathbf{1}}_{\text{stability function}} = \frac{\det(\mathbf{I} - z\mathfrak{A} + z\mathbf{1}\mathbf{b}^T)}{\det(\mathbf{I} - z\mathfrak{A})} , \quad z := \lambda h , \quad \mathbf{1} = [1, \dots, 1]^T \in \mathbb{R}^s .$$

Cramer's rule

$$\triangleright \quad S(z) = \frac{p(z)}{q(z)} , \quad p, q \in \mathcal{P}_s$$

$\hookrightarrow$ a rational function

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



$\mathcal{S}_\Psi$: implicit Euler method (11.2.13)

Impl. Euler

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

$$[\lim_{z \to \infty} S(z) = 0 !]$$

$\leftarrow$ Unbounded $\mathcal{S}_\Psi$

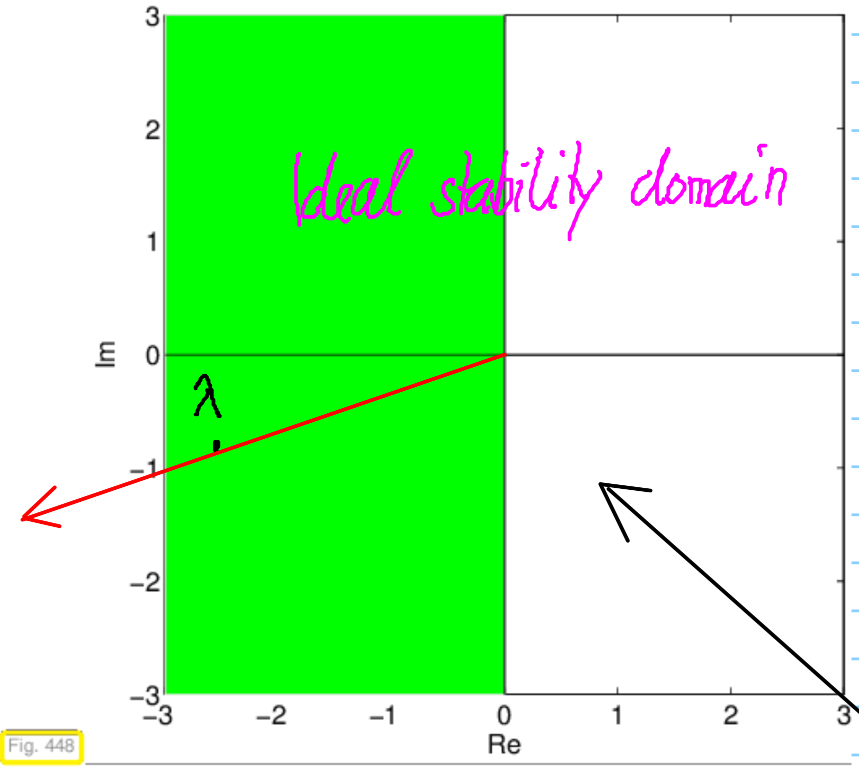


Fig. 448

$\mathcal{S}_\Psi$: implicit midpoint method (11.2.18)

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

Implicit midpoint method

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

$\Rightarrow$ Ideal stability domain:

$$\underset{\approx}{y_1} = \underset{\approx}{S(\lambda h)}\, y_0$$

$$y(h) = \underbrace{e^{\lambda h}}\, y_0$$

= "ideal stability function"

$$|e^z| = e^{\operatorname{Re} z} < 1 \Leftrightarrow \operatorname{Re} z < 0$$

$$h\lambda \in \mathcal{S}_\psi \quad \forall h > 0 \qquad [\operatorname{Re}\lambda < 0]$$

$$\Leftrightarrow \quad \{z \in \mathbb{C}, \operatorname{Re} z < 0\} \subset \mathcal{S}_\psi$$

Definition 12.3.32. A-stability of a Runge-Kutta single step method

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

$$\mathbb{C}^- := \{z \in \mathbb{C}: \operatorname{Re} z < 0\} \subset \mathcal{S}_\Psi . \quad (\mathcal{S}_\Psi \triangleq \text{region of stability Def. 12.1.49})$$