ETH Lecture 401-0674-00L Numerical Methods for ~~Partial~~ Differential Equations

Course Video

Section 7.1: Model Problem Analysis

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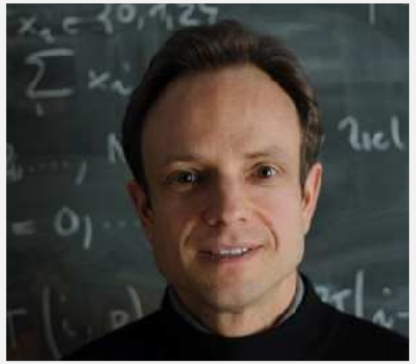


Date: April 5, 2021

Prerequisites.

- Complex numbers
- Diagonalization of matrices

Dependencies. [Lecture → Section 6.2.1], [Lecture → Section 6.4], [Lecture → Section 6.5], [Lecture → § 6.5.3.2]

Duration: minutes

Video and accompanying tablet notes may not match completely!

[Corrections and updates may have been made in tablet notes.]

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

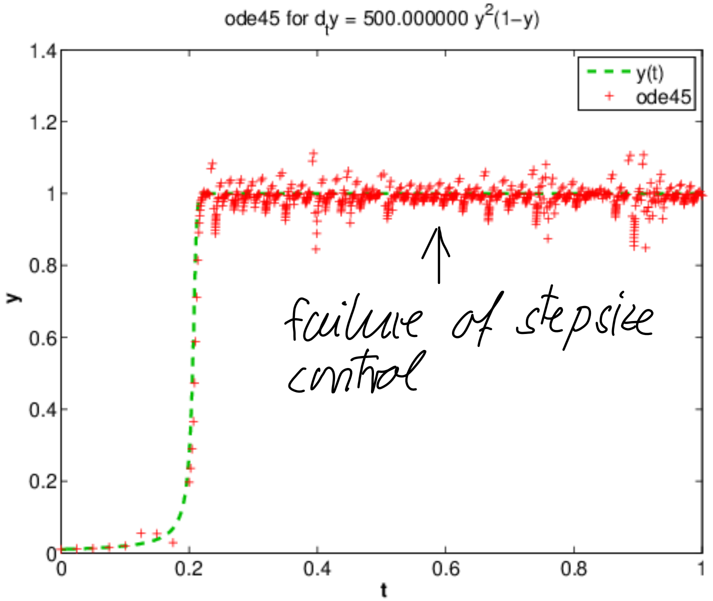
Exp. 7.0.0.1 ($\underbrace{\text{Explicit adaptive RK-SSM}}$ for stiff IVP)

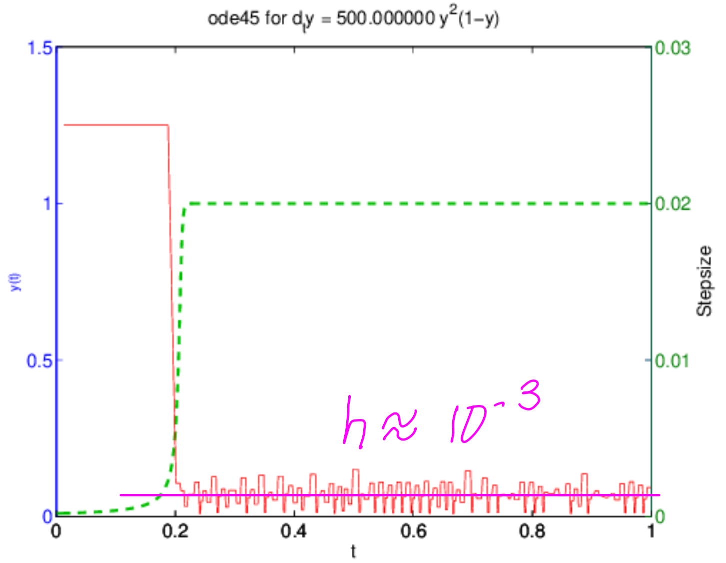
→ Sect. 6.5.3, § 6.5.3.2 : Ode45

IVP : $\dot{y} = \lambda y^2(1-y)$, $\lambda = 500$, $y(0) = 0.01$

Statistics of the integrator run ▷

1	— number of steps:	183
2	— number of rejected steps:	185
3	— function calls:	1302



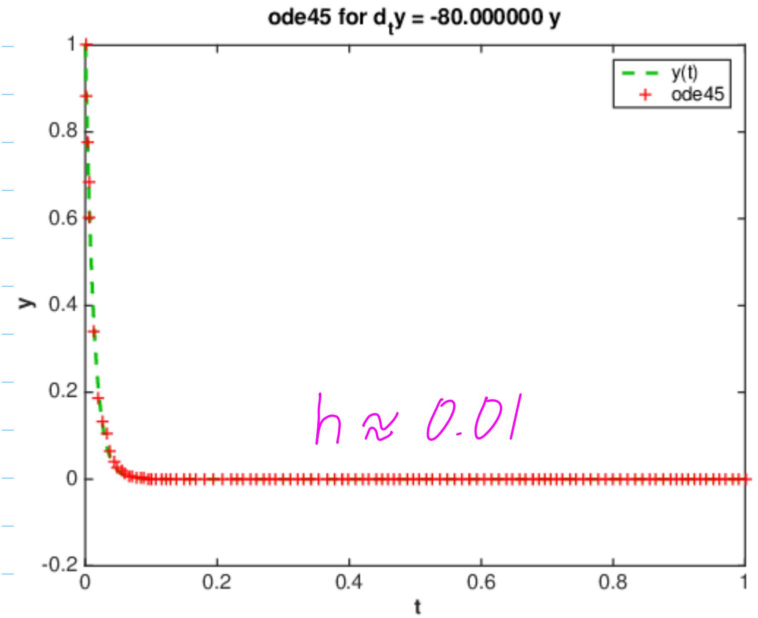


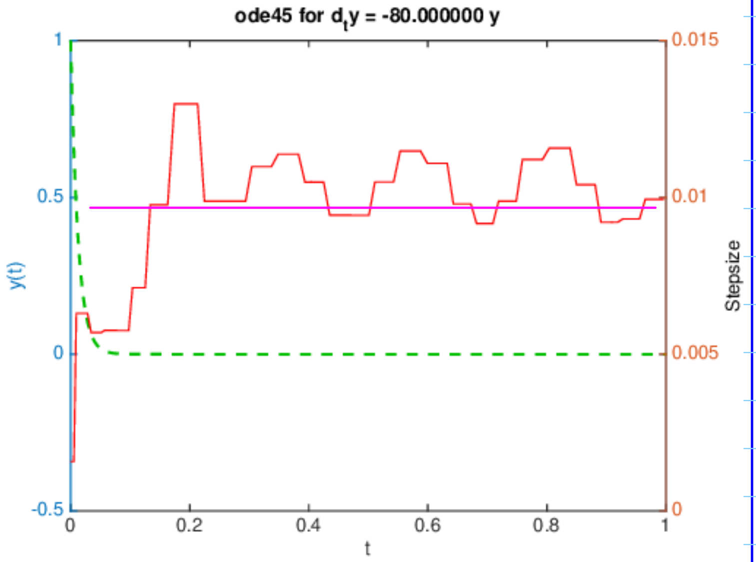
7.1. Model Problem Analysis

Exp. 7.1.0.1. (Adaptive explicit RK-SSM for scalar linear decay ODE)

↳ Ode45, § 6.5.3.2

Scalar linear IVP: $\dot{y} = \lambda y$, $\lambda = -80$, $y(0) = 1$





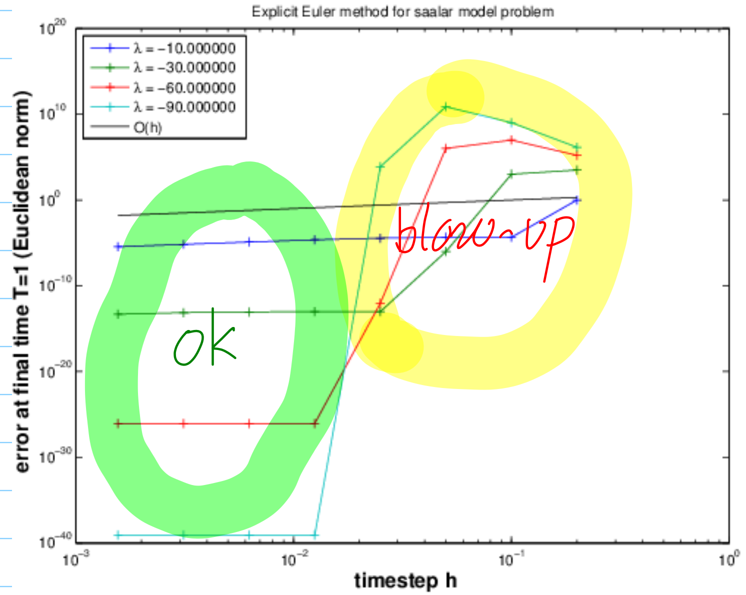
→ Unreasonably small timestep $h \approx 0.01$ to "approximate" $y(t) = 0$

Ex. 7.1.0.3 (Blow-up of explicit Euler method)

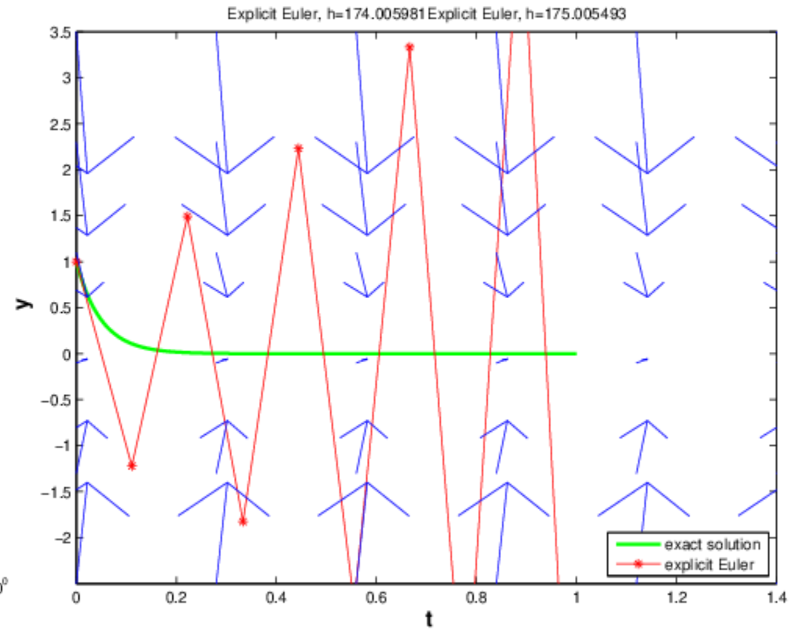
- We consider the IVP for the scalar linear decay ODE:

$$\dot{y} = f(y) := \lambda y\,, \quad \lambda \ll 0 \quad , \quad y(0) = 1\,.$$

- We apply the explicit Euler method (6.2.1.4) with uniform timestep $h = 1/N$, $N \in \{5, 10, 20, 40, 80, 160, 320, 640\}$.



$\lambda \ll 0$: blow-up of y_k for large timestep h



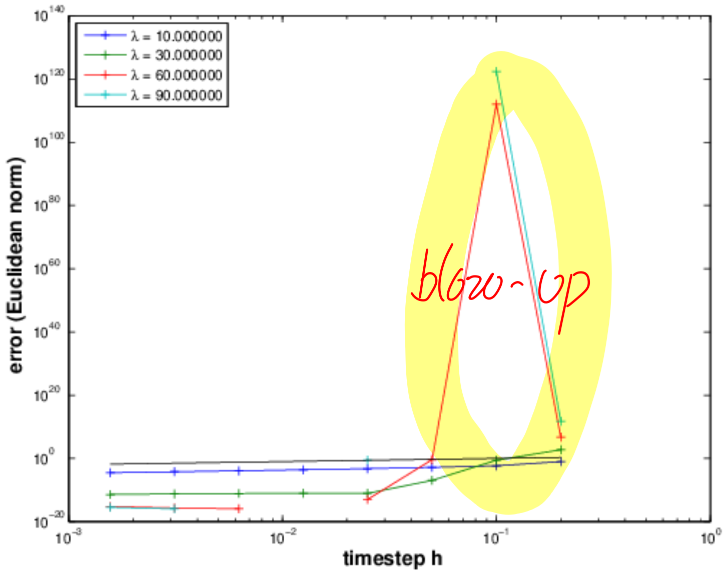
$\lambda = 20$: — $\hat{=}$ $y(t)$, — $\hat{=}$ Euler polygon

["overshooting"]

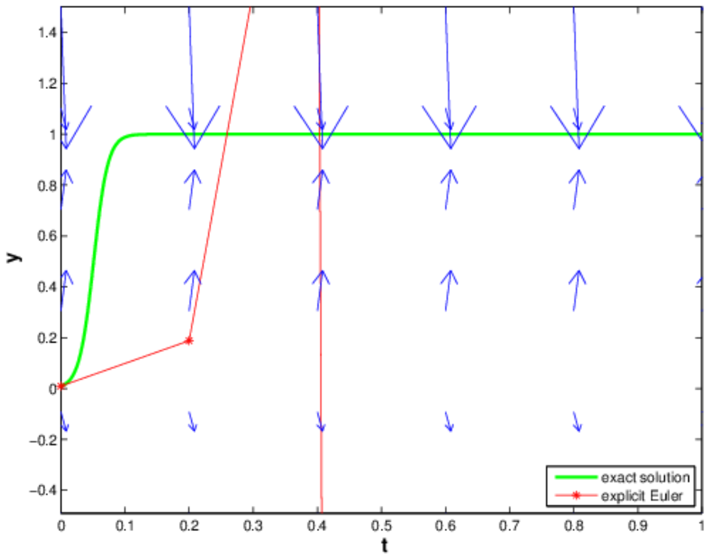
- Now we look at an IVP for the logistic ODE, see Ex. 6.1.2.1:

$$\dot{y} = f(y) := \lambda y(1 - y) \quad , \quad y(0) = 0.01\,.$$

- As before, we apply the explicit Euler method (6.2.1.4) with uniform timestep $h = 1/N$, $N \in \{5, 10, 20, 40, 80, 160, 320, 640\}$.



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



$\lambda = 90$: — $\hat{=}$ $y(t)$, — $\hat{=}$ Euler polygon

["overshoot"]

§ 7.1.0.4 (Linear model problem analysis: explicit Euler method)

Linear model problem IVP: $\dot{y} = f(y) := \lambda y$, $y(0) = y_0$, $\lambda \ll 0$

▷ Solution $y(t) = y_0 e^{\lambda t} \longrightarrow 0$ for $t \to \infty$

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

$$|y_k| = |(1+h\lambda)^k y_0| \xrightarrow{k\to\infty} \begin{cases} 0, & \text{if } |1+\lambda h| < 1 \Leftrightarrow h < \frac{2}{|\lambda|} \\ \infty, & \text{if } |1+\lambda h| > 1 \Leftrightarrow h > \frac{2}{|\lambda|} \end{cases}$$

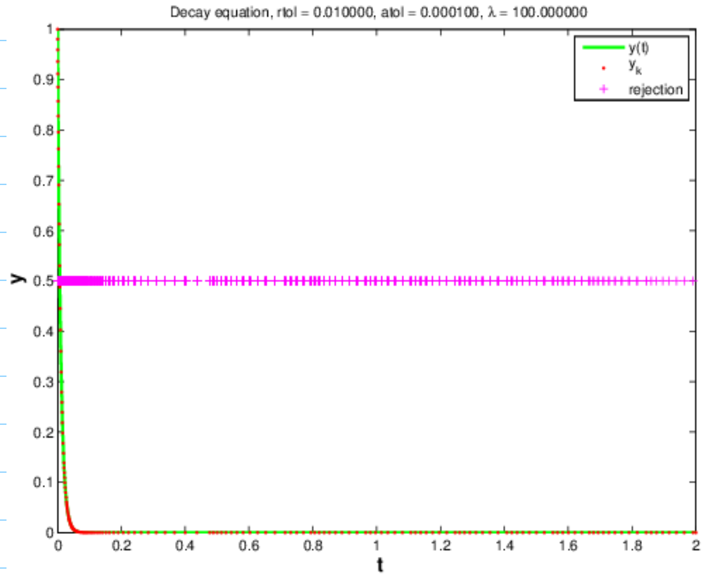
▷ Blow-up, unless $h \le \frac{2}{|\lambda|}$

$\hat{=}$ Stability-induced timestep constraint

Exp. 7.1.0.8 (Simple adaptive timestepping for fast decay)

- "Linear model problem IVP": $\dot{y} = \lambda y$, $y(0) = 1$, $\lambda = -100$
- Simple adaptive timestepping method as in Exp. 6.5.2.8, see Code 6.5.2.6. Timestep control based on the pair of 1st-order explicit Euler method and 2nd-order explicit trapezoidal method.

Timestep control based on
- explicit Euler method
- explicit trapezoidal method



◁ Stepsize control maintains timestep below stability-induced threshold.

↓

inefficient

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Ex. 7.1.0.9 (Explicit trapezoidal method for decay equation)

Explicit trapezoidal method for $\dot{y} = f(t,y)$

$$k_1 = f(t_0, y_0)\,,\quad k_2 = f(t_0+h, y_0 + hk_1)$$

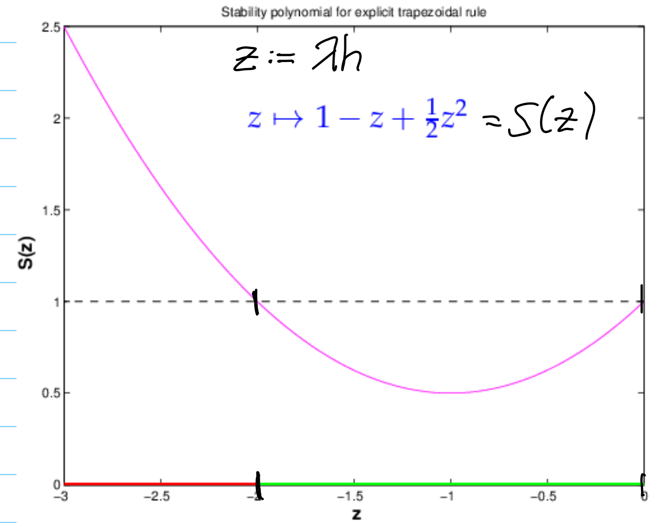
$$y_1 = y_0 + \tfrac{1}{2}h\,(k_1 + k_2)$$

For $f(t,y) := \lambda y\,,\quad \lambda < 0$:

$$k_1 = \lambda y_0\,,\quad k_2 = \lambda(y_0 + \lambda h y_0)$$

$$\Rightarrow \quad y_1 = \underbrace{\left(1 + \lambda h + \tfrac{1}{2}(\lambda h)^2\right)}_{=:\, S(\lambda h)} y_0$$

$$\Rightarrow \quad y_k = (S(\lambda h))^k \cdot y_0\,,\quad k \in \mathbb{N}$$



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

$$h \le |2/\lambda|\,. \tag{7.1.0.12}$$

◁ the **stability function** for the explicit trapezoidal method

§ 7.1.0.13 (Model problem analysis for general explicit RK-SSMs)

s-stage RK-SSM $\longleftrightarrow$ $\begin{array}{c|c} c & \mathfrak{A} \\ \hline & b^T \end{array}$, $\mathfrak{A} \in \mathbb{R}^{s,s}$ strictly lower triangular, $c, b \in \mathbb{R}^s$

Definition 6.4.0.9. 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 $\dot{\mathbf{y}} = \mathbf{f}(t,\mathbf{y})$, $\mathbf{f}: \Omega \to \mathbb{R}^N$, is defined by ($\mathbf{y}_0 \in D$)

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

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

For $N = 1$, $f(t,y) := \lambda y\,,\ \lambda \in \mathbb{R}$:

$$k_i = \lambda\Big(y_0 + h\sum_{j=1}^{i-1} a_{ij} k_j\Big)\,,$$

$$y_1 = y_0 + h\sum_{i=1}^{s} b_i k_i$$

$$\Rightarrow \quad \begin{bmatrix} \mathbf{I} - z\mathfrak{A} & 0 \\ -z\mathbf{b}^\top & 1 \end{bmatrix} \begin{bmatrix} \boldsymbol{k} \\ y_1 \end{bmatrix} = y_0 \begin{bmatrix} \mathbf{1} \\ 1 \end{bmatrix}, \tag{7.1.0.14}$$

$$\underline{k} := \tfrac{1}{\lambda}[k_1, \dots, k_s]^T \in \mathbb{R}^s$$

$$z := \lambda h$$

$$\mathbb{1} := [1, \dots, 1]^T \in \mathbb{R}^s$$

5 By Cramer's rule: $y_1 = S(\lambda h) y_0$

$$y_1 = y_0 \frac{\det\begin{bmatrix} \mathbf{I} - z\mathfrak{A} & \mathbf{1} \\ -z\mathbf{b}^\top & 1 \end{bmatrix}}{\det\begin{bmatrix} \mathbf{I} - z\mathfrak{A} & 0 \\ -z\mathbf{b}^\top & 1 \end{bmatrix}} \Rightarrow S(z) = \det(\mathbf{I} - z\mathfrak{A} + z\mathbf{1}\mathbf{b}^T)\,, \tag{7.1.0.16}$$

$\longrightarrow\; = 1$

Theorem 7.1.0.17. Stability function of explicit Runge-Kutta methods → ,

The discrete evolution Ψ^h_λ of an explicit s-stage Runge-Kutta single step method (→ Def. 6.4.0.9) with Butcher scheme $\begin{array}{c|c} \mathbf{c} & \mathfrak{A} \\ \hline & \mathbf{b}^T \end{array}$ *(see (6.4.0.11)) 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** (SF)*

$$S(z) := 1 + z\mathbf{b}^T(\mathbf{I} - z\mathfrak{A})^{-1}\mathbf{1} = \det(\mathbf{I} - z\mathfrak{A} + z\mathbf{1}\mathbf{b}^T)\,, \quad \mathbf{1} := [1,\dots,1]^\top \in \mathbb{R}^s\,. \tag{7.1.0.18}$$

↳ a polynomial of degree $\leq s$

Corollary 7.1.0.20. Polynomial stability function of explicit RK-SSM

For a consistent (→ Def. 6.3.1.11) s-stage explicit Runge-Kutta single step method according to Def. 6.4.0.9 the stability function S defined by (9.2.7.47) is a non-constant polynomial of degree $\leq s$, that is, $S \in \mathcal{P}_s$.

Ex. 7.1.0.19 (Stability functions of some explicit RK-SSMs)

Explicit Euler method (6.2.1.4): $\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$ ➤ $S(z) = 1 + z$.

Expl. trapezoidal method (6.4.0.6): $\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$ ➤ $S(z) = 1 + z + \frac{1}{2}z^2$.

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

↑ truncated exp. ser.

Rem. 7.1.0.21 (Stability function and exponential function)

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

- RK-SSM: $y_1 = S(\lambda h) \cdot y_0$
- Exact: $y(h) = e^{\lambda h} \cdot y_0$

⇒ Expect: $S(\lambda h) \approx e^{\lambda h} = \sum_{\ell=0}^{\infty} \frac{1}{\ell!} z^\ell$, $z := \lambda h$

⟹ Order q: $S(z) = \sum_{\ell=0}^{q} \frac{1}{\ell!} z^\ell + z^{q+1} p(z)$

Lemma 7.1.0.23. Stability function as approximation of $\exp$ for small arguments

Let S denote the stability function of an s-stage explicit Runge-Kutta single step method of order $q \in \mathbb{N}$. Then

$$|S(z) - \exp(z)| = O(|z|^{q+1}) \quad \text{for} \quad |z| \to 0\,. \tag{7.1.0.24}$$

↳ one-step error for $\dot{y} = \lambda y$

Corollary 7.1.0.25. Stages limit order of explicit RK-SSM

An explicit s-stage RK-SSM has maximal order $q \le s$.

§ 7.1.0.26 (Stability-induced timestep constraint)

$|S(h\lambda)| > 1 \Rightarrow$ Exp. blow-up of $(y_k)_k$ for $k \to \infty$

↳ $= S(h\lambda)^k y_0$

$S \in \mathcal{P}_s$, $S \neq \text{const} \Rightarrow \lim_{|z| \to \infty} |S(z)| = \infty$

▷ $\{z \in \mathbb{R} : |S(z)| \le 1\}$ bounded

$\Rightarrow$ $|S(h\lambda)| \le 1$ only if $|h|$ sufficiently small

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 (7.1.0.5) with uniform timestep $h > 0$,

↳ stability-induced timestep constraint

For $\lambda < 0$, $|\lambda| \gg 1$ enforces timesteps way smaller than required by accuracy: inefficient

§ 7.1.0.30 (Systems of linear ODEs)

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

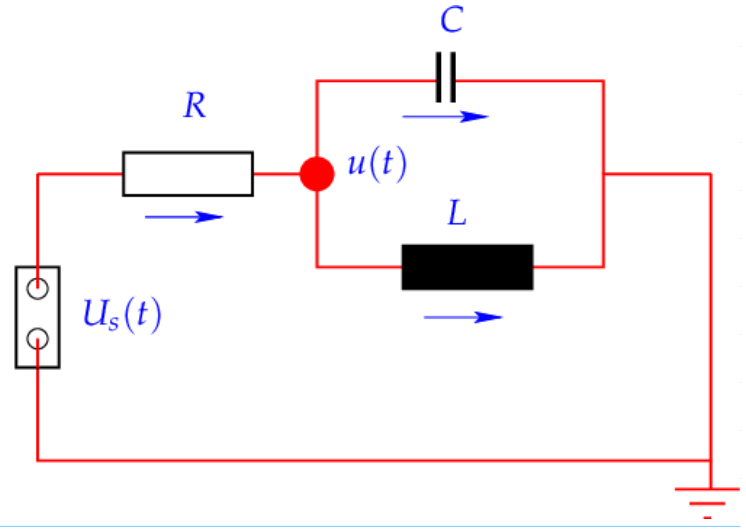
Ex. 7.1.0.35 (Transient simulation of RLC circuit)

Consider circuit from Ex. 6.1.2.9 ▷

Transient nodal analysis leads to the second-order linear ODE

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

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



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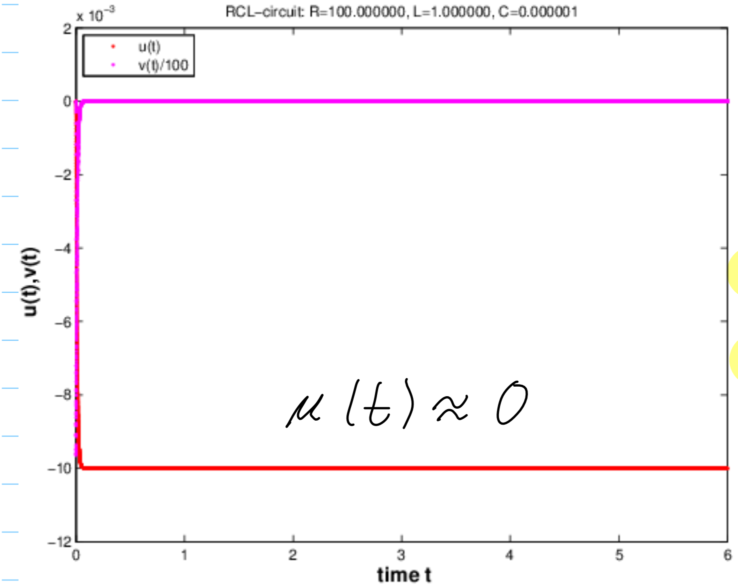
Equivalent linear (non-autonomous) first-order ODE

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

with $\beta \gg \alpha \gg 1$ in usual settings.

$\Leftrightarrow$ Affine linear ODE: $\dot{y} = My + b(t)$

Apply adaptive embedded RK-SSM Ode45:



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

ode45 statistics:

```
17901 successful steps
1210 failed attempts
114667 function evaluations
```

Tiny timesteps despite virtually constant solution!

Recalled: Diagonalization of $\dot{y} = My$

$$\exists V \in \mathbb{C}^{N,N}: \quad V^{-1}MV = D = \mathrm{diag}(\lambda_1,\dots,\lambda_N)$$

$$\dot{y} = My \quad \xRightarrow[{[z(t) = V^{-1}y(t)]}]{} \quad \dot{z} = Dy$$

$$\Updownarrow$$

Decoupled scalar ODEs $\quad \dot{z}_\ell = \lambda_\ell z_\ell, \quad \ell = 1,\dots,N$

$$z_\ell(t) = e^{\lambda_\ell t}\cdot z_\ell(0)$$

$$\Rightarrow \quad y(t) = Vz(t) = V\,\mathrm{diag}(e^{\lambda_\ell t})_{\ell=1}^{N}\, V^{-1} y(0)$$

§ 7.1.0.40 ("Diagonalization" of explicit Euler method)

$$\dot{y} = f(y) := My \quad \Rightarrow \quad y_{k+1} = y_k + hMy_k$$

$$[\exists V \in \mathbb{C}^{N,N}: \; V^{-1}MV = D = \mathrm{diag}(\lambda_1,\dots,\lambda_N)\,]$$

$$\Rightarrow \quad V^{-1}y_{k+1} = V^{-1}y_k + h\,\overbrace{V^{-1}MV}^{D}\,(V^{-1}y_k)$$

$$[z_k = V^{-1}y_k]: \quad z_{k+1} = z_k + hDz_k$$

$\Rightarrow \underbrace{(z_{k+1})_\ell = (z_k)_\ell + h\lambda_\ell (z_k)_\ell}$

$\leftrightarrow$ EE for $\dot{y} = \lambda_\ell y$

The explicit Euler method generates uniformly bounded solution sequences $(\mathbf{y}_k)_{k=0}^\infty$ for $\dot{\mathbf{y}} = \mathbf{M}\mathbf{y}$ with diagonalizable matrix $\mathbf{M} \in \mathbb{R}^{N,N}$ with eigenvalues $\lambda_1, \dots, \lambda_N$, if and only if it generates uniformly bounded sequences for **all** the scalar ODEs $\dot{z} = \lambda_i z$, $i = 1, \dots, N$.

$\hookrightarrow \ |1 + \lambda_\ell h| \leq 1$

Also applies to $\lambda_\ell \in \mathbb{C}$, Rem. 7.1.0.42

§ 7.1.0.43 (Extended model problem analysis for explicit RK-SSMs)

Definition 6.4.0.9. 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 $\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y})$, $\mathbf{f} : \Omega \to \mathbb{R}^N$, is defined by ($\mathbf{y}_0 \in D$)

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

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

$\leftrightarrow$ Butcher scheme $\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$, $A \in \mathbb{R}^{s,s}$

Apply to ODE $\dot{y} = f(y) := My$

$$\mathbf{k}_\ell = \mathbf{M}(\mathbf{y}_0 + h \sum_{j=1}^{\ell-1} a_{\ell j} \mathbf{k}_j), \quad \ell = 1, \dots, s \quad , \quad \mathbf{y}_1 = \mathbf{y}_0 + h \sum_{\ell=1}^{s} b_i \mathbf{k}_\ell . \qquad (7.1.0.44)$$

Diagonalization:

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

$\cdot V^{-1}$

$$V^{-1} k_\ell = V^{-1} M V (V^{-1} y_0 + h \sum_{j=1}^{\ell-1} a_{ij} V^{-1} k_j)$$

$$V^{-1} y_1 = V^{-1} y_0 + h \sum_{i=1}^{s} b_i V^{-1} k_i$$

$[\hat{k}_\ell := V^{-1} k_\ell, \quad z_k := V^{-1} y_k]$

$$\hat{k}_\ell = D (z_0 + h \sum_{j=1}^{\ell-1} a_{ij} \hat{k}_j)$$

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

Decoupled:

$$(\hat{k}_\ell)_m = \lambda_m ((z_0)_m + h \sum a_{ij} (\hat{k}_j)_m)$$

$$(z_1)_m = (z_0)_m + h \sum_{i=1}^{s} b_i (\hat{k}_i)_m \quad , m = 1, \dots, N$$

$\hat{=}$ RK-SSM for $\dot{y} = \lambda_m y$

The RK-SSM generates uniformly bounded solution sequences $(\mathbf{y}_k)_{k=0}^{\infty}$ for the ODE $\dot{\mathbf{y}} = \mathbf{M}\mathbf{y}$ with diagonalizable matrix $\mathbf{M} \in \mathbb{R}^{N,N}$ with eigenvalues $\lambda_1, \dots, \lambda_N$, if and only if it generates uniformly bounded sequences for **all** the scalar ODEs $\dot{z} = \lambda_i z$, $i = 1, \dots, N$.

Stability analysis: reduction to scalar case

Understanding the behavior of RK-SSM for autonomous scalar linear ODEs $\dot{y} = \lambda y$ with $\lambda \in \mathbb{C}$ is enough to predict their behavior for general autonomous linear systems of ODEs.

Note: $\|y_k\| \longrightarrow \infty$

$\Updownarrow$ for $k \to \infty$

$\exists m \in \{1,..,N\}: |(z_k)_m| \longrightarrow \infty$

Theorem 7.1.0.48. (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. 6.4.0.9) with stability function S (defined in (9.2.7.47)) applied to the linear autonomous ODE $\dot{\mathbf{y}} = \mathbf{M}\mathbf{y}$, $\mathbf{M} \in \mathbb{C}^{N,N}$, with uniform timestep $h > 0$ decays exponentially for every initial state $\mathbf{y}_0 \in \mathbb{C}^N$, if and only if $|S(\lambda_i h)| < 1$ for all eigenvalues λ_i of $\mathbf{M}$.

§ 7.1.0.49 (Region of stability for explicit RK-SSM)

Definition 7.1.0.51. Region of (absolute) stability

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

$$\Psi^h y = S(z)y\,, \quad y \in \mathbb{C}, h > 0 \quad \text{with} \quad z := h\lambda \tag{7.1.0.52}$$

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

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

$\lambda h \in \mathcal{S}_\Psi \Rightarrow$ No blow-up of RK-SSM for ODE $\dot{y} = \lambda y$

Explicit s-stage RK-SSMs: $S \in \mathcal{P}_s$, $S \neq$ const

$\Rightarrow$ $\mathcal{S}_\Psi$ bounded

$\Rightarrow$ Timestep constraint: $\lambda_m h \in \mathcal{S}_\Psi$ $\forall m = 1,..,N$

$\forall$ λ_m eigenvalue of $M \in \mathbb{R}^{N,N}$ to avoid blow-up for $\dot{y} = My$!

Please answer review questions

After you have watched the video take a short break and then try to answer the

review questions 7.1.0.54

Please avoid consulting the lecture document or tablet notes.