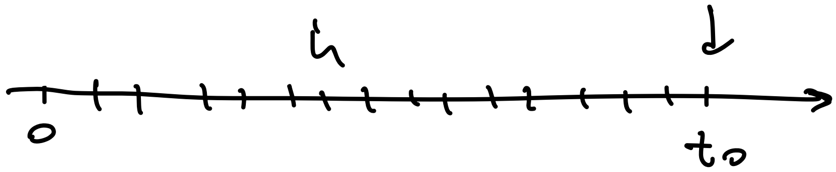
Numerical integration of ODEs

$$\begin{cases}\dot{\vec q}(t) = \vec f(\vec q(t), t) \\ \vec q(0) = \vec q_0\end{cases} \qquad \vec q \in \mathbb{R}^N$$

Numerical scheme



$M = \frac{t_0}{h}$ $\qquad$ $t_n = nh$

$$\to \vec q_{n+1} = \vec \Psi_n\big((\underset{\text{implicit}}{\vec q_{n+1}}), \vec q_n, \dots, \vec q_0; \vec f, h\big)$$

alternative formulation (more explicit)

k-step approach $\qquad$ $n=0$

let:

$$\to \sum_{j=0}^{k} \alpha_j \vec q_{n+j} = \vec \Phi_{f}\big(\vec q_n, \vec q_{n+1}, \dots, (\underset{\text{implicit}}{\vec q_{n+k}}); t_n, h\big)$$

(n+k)-th vector $\vec q_{n+k}$

Euler scheme

$$\boxed{\vec q_{n+1} = \vec q_n + h \vec f(\vec q_n, t_n) + \mathcal{O}(h^2)}$$

Consistency of a method (local error)

$\vec{y}(t_n)$ exact solution

$$\left| \vec{y}(t_{n+1}) - \vec{y}_n\left(\vec{y}(t_{n+1}), \vec{y}(t_n), \ldots, \vec{y}(0); \vec{f}, h \right) \right|$$

$$\sim O(h^{p+1})$$

consistency of order p

Convergence of a method

$$\left| \vec{y}_n - \vec{y}(t_n) \right| \sim O(h^p)$$

convergence of order p

Intuitively

$$\vec{y}_1 = \vec{y}(t_1) + O(h^{p+1})$$

$$\vec{y}_2 = \vec{y}(t_2) + 2 \times O(h^{p+1})$$

$\vdots$

$$\vec{y}_n = \vec{y}(t_n) + \underbrace{n \times O(h^{p+1})}_{t_0\, O(h^p)} \qquad n = \frac{t_0}{h}$$

In the case of Euler

if $\vec{f}$ is Lipschitz-continuous $\forall t \in [0, t_0]$

$\forall \vec{x}, \vec{q} \in \mathbb{R}^N \quad : \quad \exists L > 0$

$$\| \vec{f}(\vec{x}, t) - \vec{f}(\vec{q}, t) \| < L \| \vec{x} - \vec{q} \|$$

Euler is convergent of order $p = 1$ $\leftarrow$

time to solution of Euler

$$T = A N \frac{t_0}{h} = A' N \frac{t_0}{\epsilon}$$

accuracy of ϵ

$$| \vec{q}_n - \vec{q}(t_n) | < \epsilon$$

$\sim o(h)$

$\epsilon \sim h$

progress : $\begin{cases} 1) \boxed{\begin{array}{c} \epsilon = h^p \\ h \sim \epsilon^{1/p} \end{array}} \\ 2) \; A' \quad ? \end{cases}$

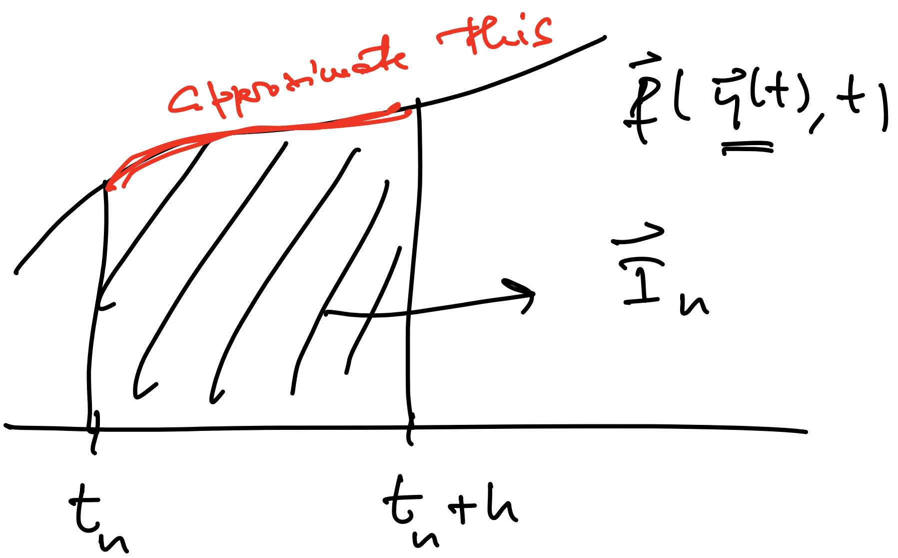
method convergent of order p

↪ method-dependent

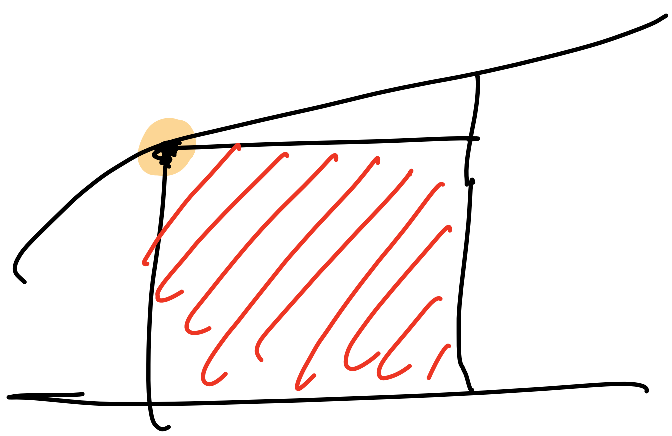
$$T \simeq \underset{=}{A}' \sim \frac{t_0}{\epsilon^{1/p}}$$

Developing $\begin{cases} \text{higher-order methods} \\ \text{implicit methods} \end{cases}$

$$\vec{\eta}(t_{n+1}) = \vec{\eta}(t_n) + \vec{I}_n$$

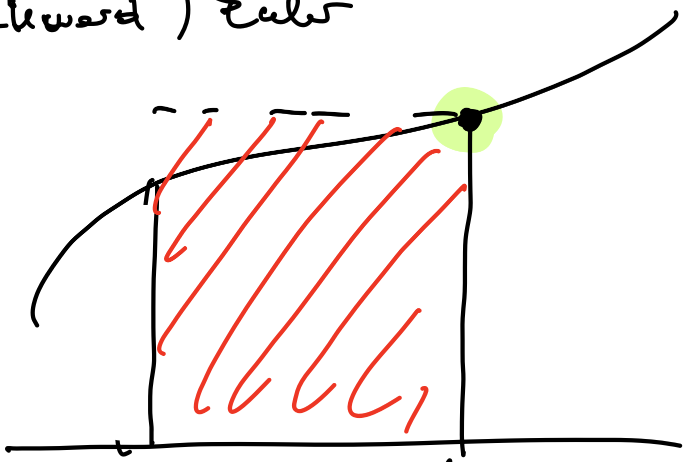


(forward) Euler

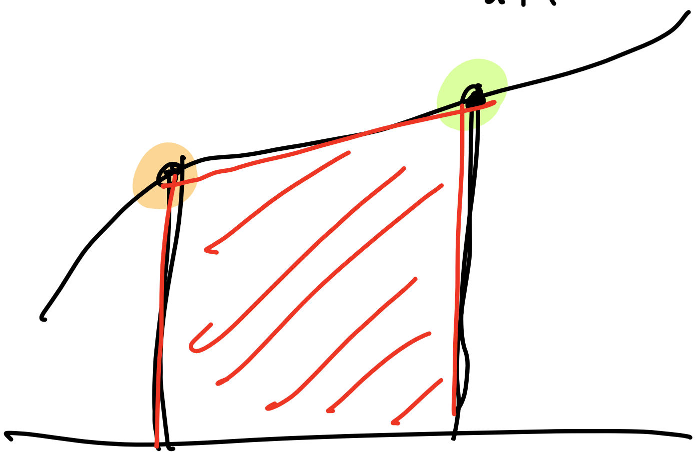


(Backward) Euler

implicit



t_{n+1}



trapezoid scheme

translating into methods

f. Euler : $\vec{y}_{n+1} = \vec{y}_n + h\,\vec{f}(\vec{y}_n, t_n) + O(h^2)$

b. Euler : $\vec{y}_{n+1} = \vec{y}_n + h\,\vec{f}(\vec{y}_{n+1}, t_{n+1}) + O(h^2)$

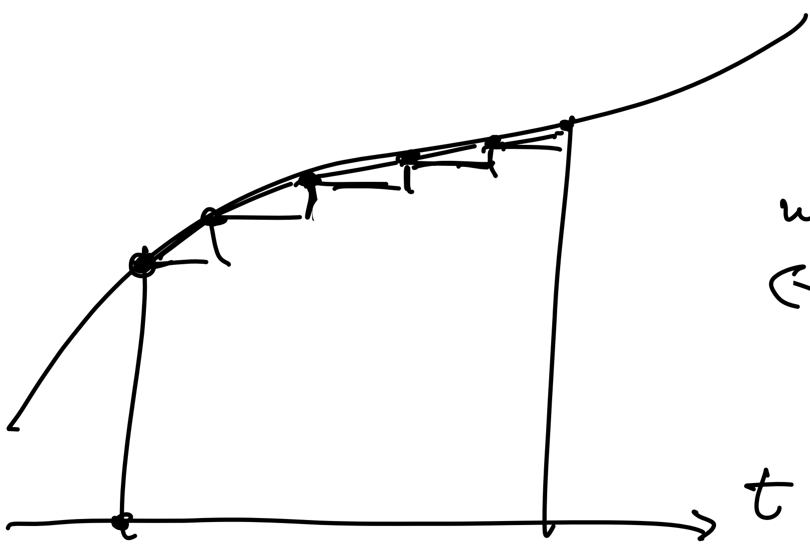
trapezoid : $\vec{y}_{n+1} = \vec{y}_n + \frac{h}{2}\left[\vec{f}(\vec{y}_n, t_n) + \vec{f}(\vec{y}_{n+1}, t_{n+1})\right] + O(h^3)$

$$\Longleftarrow$$

$$\vec{y}_n + \frac{h}{2}\left[\vec{f}(\vec{y}_n, t_n) + \vec{f}(\vec{y}_n, t_n) + h\,\frac{d\vec{f}}{dt}(\vec{y}_n, t_n) + O(h^2)\right]$$

$$= \vec{y}_n + h\,\vec{f}(\vec{y}_n, t_n) + \underbrace{\frac{h^2}{2}\frac{d\vec{f}}{dt}(\vec{y}_n, t_n)} + O(h^3)$$

Runge – Kutta methods $\rightarrow$ RK



m points

(explicit)
RK scheme with m stages

m RK vectors

$$\Rightarrow \vec{k}_1 = h\,\vec{f}(\vec{y}_n \cancel{+ a_{11}\vec{k}_1}, t_n) \qquad \text{Euler increment}$$

$$\vec{k}_2 = h\,\vec{f}(\vec{y}_n + a_{21}\vec{k}_1,\ t_n + c_2 h)$$

$$\vec{k}_3 = h\,\vec{f}(\vec{y}_n + a_{31}\vec{k}_1 + a_{32}\vec{k}_2,\ t_n + c_3 h)$$

$$\vdots$$

$$\vec{k}_m = h\,\vec{f}(\vec{y}_n + a_{m1}\vec{k}_1 + \dots + a_{m\,m-1}\vec{k}_{m-1},\ t_n + c_m h)$$

$$\vec{y}_{n+1} = \vec{y}_n + \sum_{i=1}^{m} b_i \vec{k}_i$$

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1m} \\ c_2 & a_{21} & a_{22} & \cdots & \vdots \\ \vdots & \vdots & \vdots & & \vdots \\ c_m & a_{m1} & a_{m2} & \cdots & a_{mm} \\ \hline & b_1 & b_2 & \cdots & b_m \end{array}$$

Butcher's tableau

explicit methods: the only non-zero elements

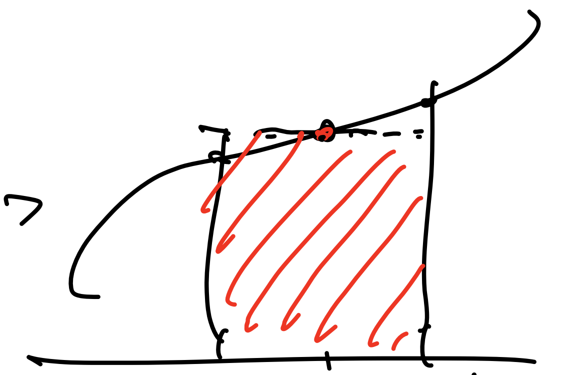
forward Euler

$$\begin{array}{c|c} 1 & 0 \\ \hline & 1 \end{array}$$

$m = 1$

order 1

mid point method



$$\Rightarrow \vec{k}_1 = h \vec{f}(\vec{y}_n, t_n)$$

$$\vec{k}_2 = h \vec{f}\Big(\underbrace{\vec{y}_n + \overset{a_{21}}{\frac{\vec{k}_1}{2}}}_{\vec{y}(t_n + \frac{h}{2})}, t_n + \frac{h}{2}\Big)$$

$$\vec{y}_{n+1} = \vec{y}_n + \vec{k}_2$$

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 0 & 1 \end{array}$$

$m=2$ method $\Rightarrow$ $p=2$ method

RK 4 $m=4$ methods

$\rightarrow$ $p=4$

$$
\begin{cases}
\vec{k}_1 = h\vec{f}(\vec{y}_n, t_n) & \text{f\_Euler} \\
\vec{k}_2 = h\vec{f}\left(\vec{y}_n + \frac{\vec{k}_1}{2}, t_n + \frac{h}{2}\right) & \text{midpoint} \\
\vec{k}_3 = h\vec{f}\left(\vec{y}_n + \frac{\vec{k}_2}{2}, t_n + \frac{h}{2}\right) & \text{midpoint ++} \\
\vec{k}_4 = h\vec{f}(\vec{y}_n + \vec{k}_3, t_n + h) & \text{"b. Euler" with } y_{n+1} = y_n + \vec{k}_3
\end{cases}
$$

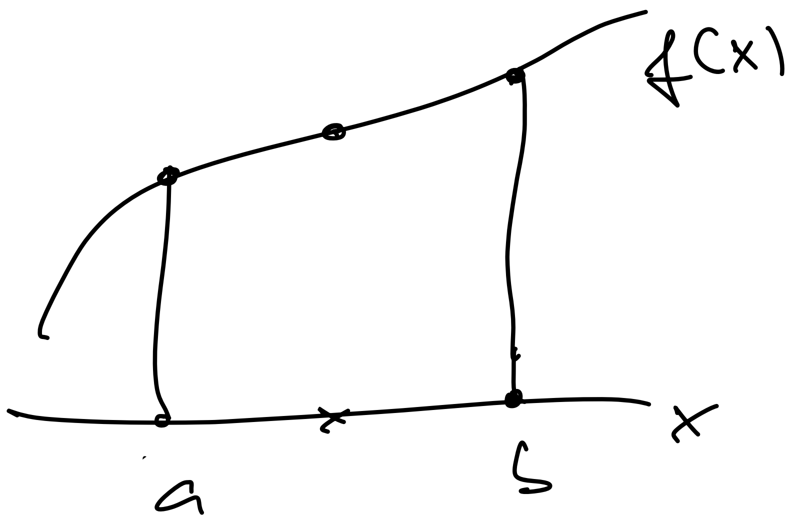
$$
\vec{y}_{n+1} = \vec{y}_n + \frac{1}{6}\left(\vec{k}_1 + 2\vec{k}_2 + 2\vec{k}_3 + \vec{k}_4\right)
$$

$$\mathcal{O}(h^5)$$

RK m-stage methods can be of order $p=m$ only up to $\underline{m=4}$

Geometrical intuition : method of numerical integration of functions

Simpson's $\frac{1}{3}$-rule



$$\int_a^b f(x)\,dx = \frac{b-a}{6}\left[f(a) + 4 f\left(\frac{a+b}{2}\right) + f(b)\right] + O(b-a)^5$$

Implicit RK methods

B. Euler

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

Implicit mid-point

$$\vec{k}_1 = h\,\vec{f}\left(\vec{y}_n + \frac{\vec{k}_1}{2},\ t_n + \frac{h}{2}\right)$$

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

$$\vec{y}_{n+1} = \vec{y}_n + \vec{k}_1$$

<u>Stability</u> : robustness of a numerical method to numerical <u>accuracy</u>

<u>Stable Cauchy problem</u>

$$\begin{cases} \dot{\vec{y}}(t) = \vec{f}(\vec{y}, t) \\ \vec{y}(0) = \vec{y}_0 \end{cases} \qquad \begin{cases} \dot{\vec{z}}(t) = \vec{f}(\vec{z}, t) + \underline{\underline{\vec{\delta}(t)}} \\ \vec{z}(0) = \vec{y}_0 + \vec{\delta}_0 \end{cases}$$

$$|\vec{\delta}(t)| < \underline{\underline{\epsilon}} \qquad \forall t$$

$$|\vec{\delta}_0| < \underline{\underline{\epsilon}}$$

C.P. is stable if $\exists\, C > 0$:

$$|\vec{z}(t) - \vec{y}(t)| < C\epsilon$$

Stability of numerical methods: zero-stability

method : k-step operation

$$\sum_{j=0}^{k} \alpha_j \vec{q}_{n+j} = h \, \vec{\Phi}_{\vec{f}}\left((\vec{q}_{n+k}), \dots \vec{q}_n; h, t_n\right)$$

to even start

$$\begin{cases} \vec{q}_0, \vec{q}_1, \dots, \vec{q}_{k-1} \\ \vec{z}_0, \vec{z}_1, \dots, \vec{z}_{k-1} \end{cases}$$

perturbed initial conditions

$$\vec{z}_j = \vec{q}_j + \vec{\delta}_j$$

perturbed method

$$\sum_{j=0}^{k} \alpha_j \vec{z}_{n+j} = h \left[\vec{\Phi}\left((\vec{z}_{n+j}), \dots, \vec{z}_n; t_n, h\right) + \vec{\delta}_{n+k} \right]$$

Method is zero-stable if:

$$|\vec{\delta}_j| < \epsilon \quad \forall j = 0, \dots, n+k$$

$$\Rightarrow \exists S > 0 : \forall j \quad |\vec{z}_j - \vec{q}_j| < S\epsilon$$

Fundamental theorem of numerical analysis

(Lax – Richtmeyer theorem)

method • consistent of order p • zero – stable	$\Longleftrightarrow$	convergent of order p

Proof of zero-stability

$$\sum_{j=0}^{k} \alpha_j \vec{q}_{n+j} = h \vec{\Phi}_{\vec{f}}\left((\vec{q}_{n+k}, \ldots \vec{q}_n; h, t_n\right)$$

(explicit)

e.g. RK methods

$$\vec{q}_{n+1} = \underline{\underline{\vec{q}_n}} + h \sum_i b_i \vec{k}_i$$

$$\vec{q}_{n+1} - \vec{q}_n = \vec{\Phi}(\qquad) \qquad \vec{k}_i = \vec{k}_i(\underline{\underline{\vec{q}_n}})$$

$k = 1$ – step method

$$\begin{cases} \alpha_0 = -1 \\ \alpha_1 = 1 \end{cases}$$

characteristic polynomial

$$p(x) = \sum_{j=0}^{k} \alpha_j \, x^j$$

RK : $p(x) = x - 1$

<u>Root condition</u> :

all the roots of $p(x)$ are such that $|x_r| \le 1$ and roots with $|x_r| = 1$ are simple $\Longrightarrow$ method is zero-stable

$$\cancel{(x_r - 1)^2}$$

RK : $x_r = 1$ ✓

"Stiff" ODEs

stiff : ODEs that require an especially small time step

Example : $\dot{y} = -ay \qquad a > 0$

$$y(t) = y(0)\, e^{-at}$$

f. Euler : $y_{n+1} = y_n - hay_n = (1-ha)y_n$

$$= (1-ha)^2 y_{n-1}$$

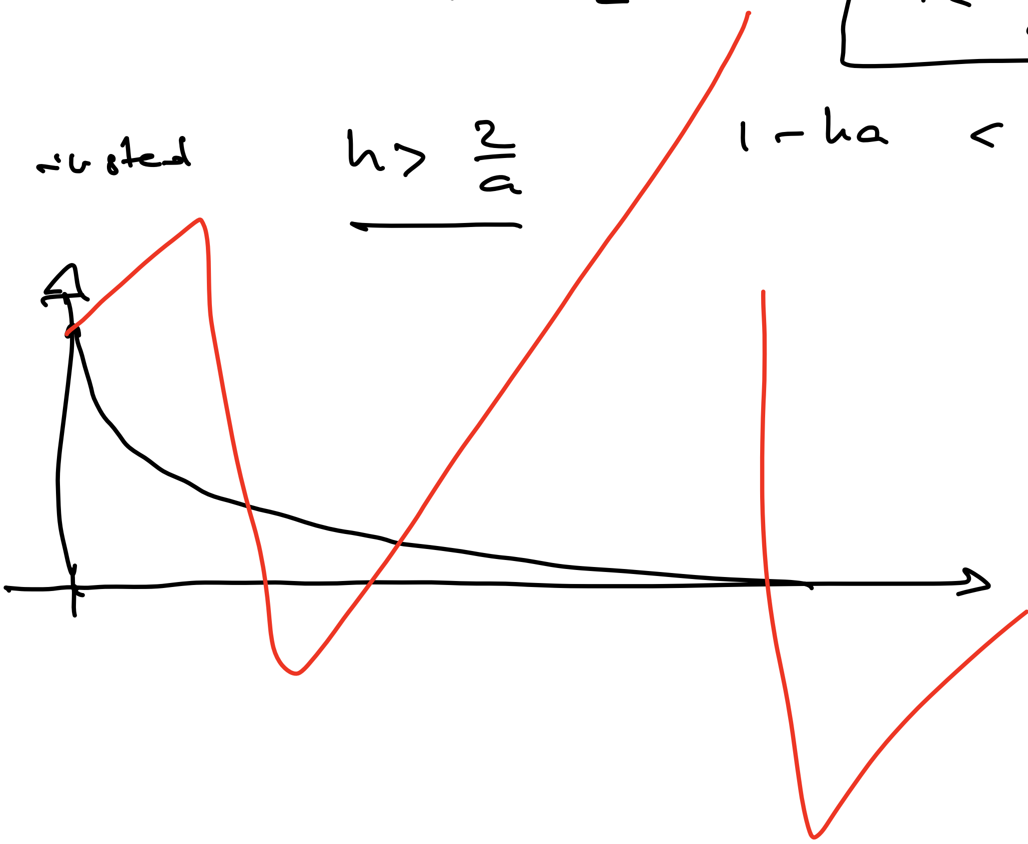
$$\cdots = (1-ha)^{n+1} y_0$$

$(1-ha)^{n+1}$ is exp. decaying with n

only if $|1-ha| < 1$

$ha < 2 \qquad \boxed{h < \frac{2}{a}}$

if violated $h > \frac{2}{a}$ $\qquad 1 - ha < -1$



b. Euler (implicit)

$$y_{n+1} = y_n - ha\, y_{n+1}$$

$$y_{n+1} = \frac{y_n}{1+ha} = \dots = \frac{y_0}{(1+ha)^{n+1}}$$

$h, a >> \quad \dfrac{1}{(1+ha)^{n+1}}$ is exp. small

$\forall h$

A- stability

Cauchy problem $\begin{cases} \dot{y}(t) = \overset{-a}{\lambda} y \\ y(0) = 1 \end{cases}$

$\rightarrow \underline{\lambda \in \mathbb{C}}$

Linear stability $\mathcal{D}$omain of a method:
values of h and λ : $y_n \xrightarrow[n \to \infty]{} 0$

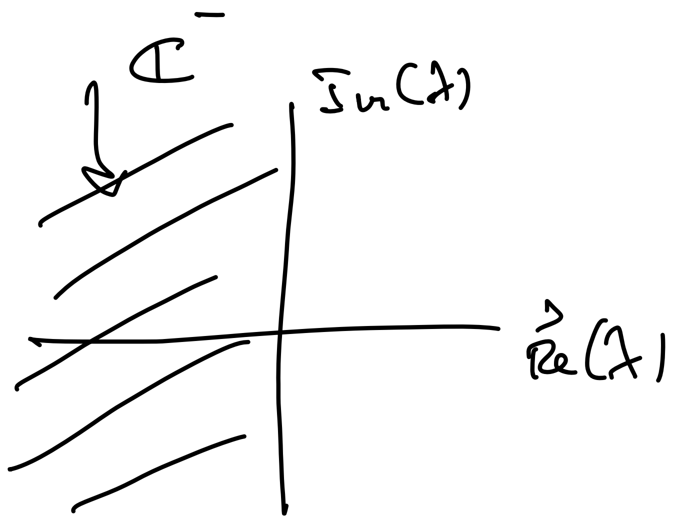
Forward Euler

$$\mathcal{D}_{FE} = \{ h, \lambda \mid |1+h\lambda| < 1 \}$$

Backward Euler

$$\mathcal{D}_{BE} = \{ h, \lambda \mid |1 - h\lambda| > 1 \}$$

Method is A-stable if



$$\mathbb{C}^- \subseteq \mathcal{D}$$

B.E is A-stable

1) No explicit RK methods are A-stable

2) Gauss-Legendre RK methods are A-stable

- Backward Euler
- implicit midpoint
- ...