Semi-discretised problem: Method of lines

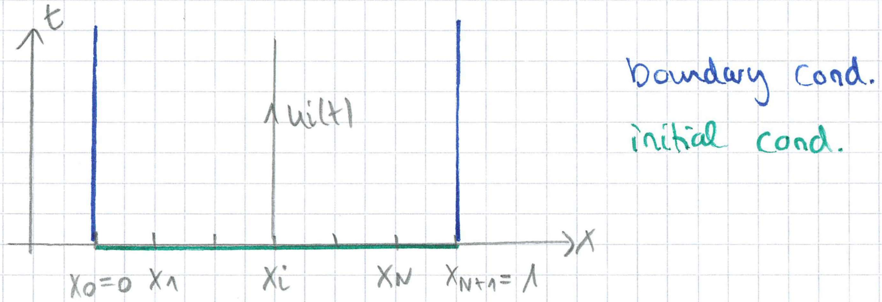
1) Discretise $[0,1]$ with $0 = x_0 < x_1 < \dots < x_{N+1} = 1$
such that $x_n = n \cdot \Delta x$

2) let $u_i(t) = u(x_i, t)$, $v_i(t) = v(x_i, t)$

3) Recall:

$$\frac{\partial^2 u}{\partial x^2}(x_i, t) = \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

with $\Delta x = \frac{1}{N+1}$.



Rewrite the ODE corresponding to the PDE:

let $y(t) = \begin{pmatrix} u_1(t) \\ \vdots \\ u_N(t) \\ v_1(t) \\ \vdots \\ v_N(t) \end{pmatrix}$

Then

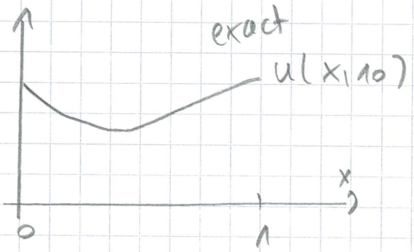
$$y'(t) = \overset{\text{constant term \& B.C.}}{g_0} + \underset{\text{linear terms}}{g_1(y)} + \frac{\nu}{\Delta x^2} \underset{\text{diffusive}}{\begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix}} y + \overset{\text{nonlinear terms}}{f(y)}$$

where $A = \begin{pmatrix} -2 & 1 & & 0 \\ 1 & -2 & 1 & \\ & 1 & \ddots & \ddots \\ 0 & & 1 & -2 \end{pmatrix}$ (comes from $\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$).

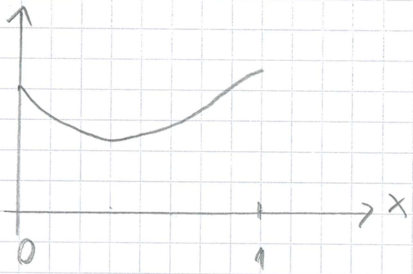
(we have an ODE and can apply numerical methods)

Numerical methods:

$t=10$

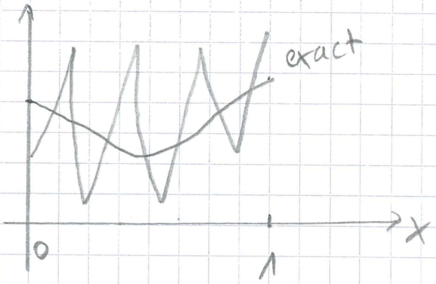


Explicit Euler:



$\Delta t < \frac{\Delta x^2}{2\omega}$

fine behaviour



$\Delta t > \frac{\Delta x^2}{2\omega}$

$\Rightarrow$ severe time stepsize restriction if Δx small

Implicit Euler:

OK for any time stepsize, <u>but</u> one has to solve large linear systems at each step.

↑(need efficient linear solver, e.g. Newton method)

Rem: see complement Brusselator with numerical illustrations.

2. Linear stability

Defn.: (Lyapunov-stable and asymptotically stable)

Consider $y'(t) = f(t,y)$, $y(t_0) = y_0$.
Then the problem is Lyapunov-stable if $\forall \varepsilon > 0 \ \exists \delta > 0$ s.t.

$\forall \Delta y_0$ s.t. $\|\Delta y_0\| < \delta$ it holds for all $t >= t_0$

$$\|\varphi_t(y_0) - \varphi_t(y_0 + \Delta y_0)\| < \varepsilon. \qquad (\varphi_t\text{: exact flow})$$

Moreover, if

$$\lim_{t \to \infty} \|\varphi_t(y_0) - \varphi_t(y_0 + \Delta y_0)\| = 0$$

then the ODE is asymptotically stable.

Linear case: $y' = Ay$, $A \in \mathbb{R}^{d \times d}$

If $y, \tilde{y}$ are both solutions, define $w = y - \tilde{y}$:

$$w' = y' - \tilde{y}' = A(y - \tilde{y}) = A w$$

$\Rightarrow$ w solves $w' = Aw$.

① A diagonalisable: $A = P \Lambda P^{-1}$ with $\Lambda = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_d \end{pmatrix}$

$\Rightarrow w' = P \Lambda P^{-1} w$

$\Rightarrow z' = \Lambda z$, $z = P^{-1} w$ $\Rightarrow \begin{cases} z_1'(t) = \lambda_1 z_1(t) \\ \vdots \\ z_d'(t) = \lambda_d z_d(t) \end{cases}$

$\Rightarrow z_i(t) = e^{\lambda_i t} z_i(0)$

$\Rightarrow \lim_{t \to \infty} |z(t)| = 0 \iff \operatorname{Re}(\lambda_i) < 0$, $i = 1, 2, \dots, d$

↳ asymptotic stability

$|z(t)| < \varepsilon \impliedby \operatorname{Re}(\lambda_i) \leq 0$, $i = 1, 2, \dots, d$

↳ Lyapunov stability.

② A non-diagonalisable: $A = PJP^{-1}$ ↑ Jordan form

$\Rightarrow w(t) = e^{tA} w_0 = P e^{tJ} P^{-1} w_0$

$\Rightarrow$ results are similar to the linear case.

Nonlinear case: Consider $y' = f(t,y)$ and two solutions $y(t), \tilde{y}(t)$ "close", $w(t) = y(t) - \tilde{y}(t)$.

$$y'(t) = f(t, y(t)) = f(t, \tilde{y}(t) + w(t))$$

$$= \underbrace{f(t, \tilde{y}(t))}_{= \tilde{y}'(t)} + \underbrace{\frac{\partial f}{\partial y}(t, \tilde{y}(t))}_{= A(t)} w(t) + \mathcal{O}(\|w(t)\|^2)$$

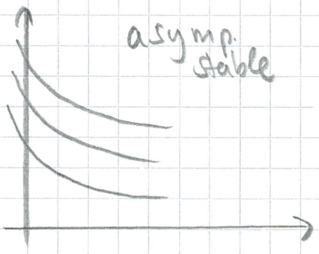
Let $A(t) = \frac{\partial f}{\partial y}(t, \tilde{y}(t))$, t small $\Rightarrow A(t) \approx A(t_0) = A$

$w(t)$ small $\Rightarrow \mathcal{O}(\|w(t)\|^2) \ll 1$.

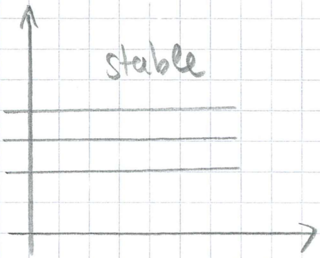
$\Rightarrow w'(t) = A\,w(t)$ -> linear.

Conclusion: Here we justified that in the following we only consider the Dahlquist test equation (1963)

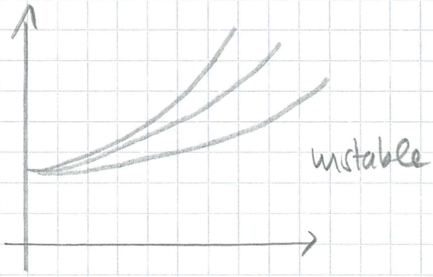
$$\boxed{\begin{cases} y' = \lambda y \\ y(0) = y_0 \end{cases}, \lambda \in \mathbb{C}}$$



Re $\lambda < 0$



Re $\lambda = 0$



Re $\lambda > 0$

Numerical stability

$$(*) \begin{cases} y' = \lambda y \\ y(0) = y_0 \end{cases}$$ Test problem

$\|y(t)\|$ bounded, if $\lambda \in \mathbb{C}^- = \{ z \in \mathbb{C} \mid Re(z) \leq 0 \}$.

What about RK methods?

Defn.: (Stability domain)

Stability domain of a RK method for $(*)$

$$S = \{ z = h\lambda \in \mathbb{C} \mid \|y_n\| \text{ remains bounded} \}.$$

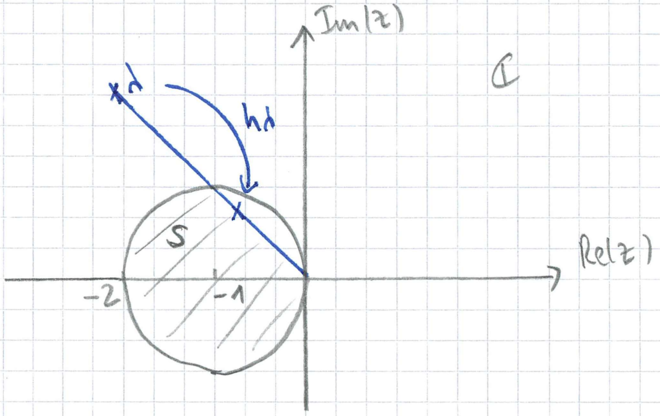
Examples:

① **Explicit Euler:**

$$y_{n+1} = y_n + h\lambda y_n = (1+h\lambda) y_n = \dots = (1+h\lambda)^{n+1} y_0$$

$$\Rightarrow \|y_n\| \text{ bounded} \iff |1+\underbrace{h\lambda}_{=z}|^n \leq 1$$

$$\Rightarrow \underline{\underline{S = \{ |1+z| \leq 1 \}}}$$



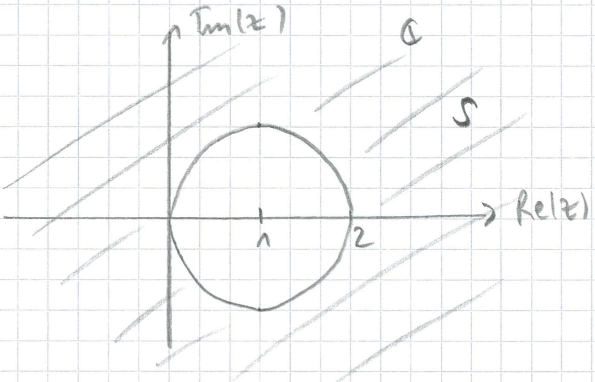
$$\Rightarrow \text{step size restriction: } |1+h\lambda| \leq 1 \Rightarrow h \leq \frac{2}{|\lambda|}$$

② Implicit Euler:

$$y_{n+1} = y_n + h\lambda \, y_{n+1}$$

$$\Rightarrow y_{n+1} = \left(\frac{1}{1-h\lambda}\right)^{n+1} y_0$$

$$\Rightarrow \text{stability} \Leftrightarrow 1 \leq |1-h\lambda|$$



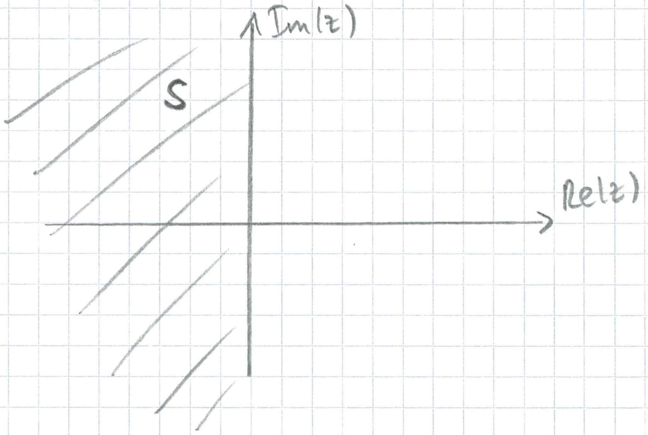
$\Rightarrow$ no step size restriction.

③ Implicit midpoint rule: (implicit trapezoidal rule)

$$y_{n+1} = y_n + \frac{h\lambda}{2}(y_n + y_{n+1})$$

$$\Rightarrow y_{n+1} = \left(\frac{1+\frac{h\lambda}{2}}{1-\frac{h\lambda}{2}}\right)^{n+1} y_0$$

$$\Rightarrow \text{stability} \Leftrightarrow |2+h\lambda| \leq |2-h\lambda|$$



Dahlquist, 1963

Defn.: (A-stable)

A RK method is A-stable

$\Longleftrightarrow \quad S \supset \mathbb{C}^- = \{ z \in \mathbb{C} \mid \mathrm{Re}(z) \leq 0 \}$

Rem.: Explicit Euler not A-stable.
Implicit Euler & implicit midpoint rule A-stable.

Defn.: (stiff ODE)
not universal

A stable ODE $y' = f(t,y)$ is stiff, when $\max_i |\mathrm{Re}(\lambda_i)|$ is large, where λ_i is an eigenvalue of $\frac{\partial f}{\partial y}$, evaluated at some point $(\hat{t}, \hat{y})$.

The value $L = \max_i |\mathrm{Re}(\lambda_i)|$ is sometimes called stiffness index.

Rem.: There exist stiff ODEs which have large almost imaginary eigenvalues, e.g. Van der Pol equation.

3. Stability functions of RK methods

Lemma 1: Consider a s-stage RK method with coefficients (b_i, a_{ij}) applied to $y' = \lambda y$.

Then $y_1 = R(h\lambda) y_0$,

where $R(z) = 1 + z b^T (I - z \mathcal{A})^{-1} \mathbb{1}$

with $(\mathcal{A})_{ij} = a_{ij}$, $b = (b_1, \dots, b_s)^T$, $\mathbb{1} = (1, \dots, 1)^T$.

Proof: let $g_i = y_0 + h \sum_{j=1}^{s} a_{ij} k_j$

$\rightarrow k_i = f(g_i)$

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

$$\overset{y'=\lambda y}{\Longrightarrow} \quad g_i = y_0 + h \sum_{j=1}^{s} a_{ij} \lambda g_j$$

$$= y_0 + h\lambda (\mathcal{A} g)_i \quad \text{, where } g = (g_1, \dots, g_s)^T$$

$$\Rightarrow \quad g = y_0 \mathbb{1} + h\lambda \mathcal{A} g$$

$$\Rightarrow \quad g = (I - h\lambda \mathcal{A})^{-1} \mathbb{1} y_0$$

Thus, $y_1 = y_0 + h\lambda \sum_{i=1}^{s} b_i g_i$

$$= y_0 + h\lambda b^T g$$

$$= \Big(\underbrace{1 + b^T h\lambda (I - h\lambda \mathcal{A})^{-1} \mathbb{1}}_{= R(h\lambda)} \Big) y_0 \quad . \quad \#$$

Defn.: (stability function)

Since $y_n = R(h\lambda)^n y_0$, we call stability function of the method the function $R(z)$.

In addition, we redefine the stability region S as

$$S = \{ z \in \mathbb{C} : |R(z)| \leq 1 \}.$$

Lemma:

The stability function of a RK method can be expressed as

$$R(z) = \frac{P(z)}{Q(z)}, \quad \text{where } P, Q \text{ are}$$

polynomials of degree $\leq s$ given by

$$P(z) = \det(I - z(\mathcal{A} - \mathbb{1} b^T))$$

$$Q(z) = \det(I - z\mathcal{A}).$$

Proof: Recall

1) $R(z) = 1 + z b^T \overbrace{(I - z\mathcal{A})^{-1} \mathbb{1}}^{g}$

2) $g = (I - z\mathcal{A})^{-1} \mathbb{1}$ $\quad (y_0 = 1)$

$$\Rightarrow \begin{cases} (I - z\mathcal{A}) g = \mathbb{1} \\ R(z) - z b^T g = 1 \end{cases}$$

rewriting

$$\left(\begin{array}{ccc|c} & I - z\mathcal{A} & & \begin{matrix} 0 \\ \vdots \\ 0 \end{matrix} \\ \hline -zb_1 & \cdots & -zb_s & 1 \end{array}\right) \left(\begin{array}{c} g \\ \hline R(z) \end{array}\right) = \left(\begin{array}{c} 1 \\ \vdots \\ 1 \end{array}\right) \quad \text{(linear system)}$$

Cramer's rule $\Longrightarrow$

$$R(z) = \frac{\det \left(\begin{array}{ccc|c} & I - z\mathcal{A} & & \overset{\text{"}Ax=b\text{"}\ \partial b}{\downarrow} \\ & & & 1 \\ & & & \vdots \\ & & & 1 \\ \hline -zb_1 & \cdots & -zb_s & 1 \end{array}\right) =: P(z)}{\det \left(\begin{array}{ccc|c} & I - z\mathcal{A} & & 0 \\ & & & \vdots \\ & & & 0 \\ \hline -zb_1 & \cdots & -zb_s & 1 \end{array}\right) = \det(I - z\mathcal{A}) = Q(z)}$$

Observe that (subtracting the last row to all other rows)

$$P(z) = \det \left(\begin{array}{ccc|c} & I - z\mathcal{A} + z\mathbb{1}b^T & & 0 \\ & & & \vdots \\ & & & 0 \\ \hline -zb_1 & \cdots & -zb_s & 1 \end{array}\right)$$

$$= \det(I - z\mathcal{A} + z\mathbb{1}b^T).$$

#

Corollary: The stability function of an explicit RK method is a polynomial.

Proof: $Q(z) = \det(I - z\mathcal{A}) = \det \begin{pmatrix} 1 & & 0 \\ & \ddots & \\ -za_{ij} & & 1 \end{pmatrix} = \underline{\underline{1}}$ #

Corollary: No consistent explicit method is A-stable.

Proof: $|P(z)| \to \infty$ for $z \to -\infty$.

($\mathbb{C}^-$ not a subset of S)

Remarks:

1) Two different RK methods can have the same stability function, e.g. implicit midpoint rule and implicit trapezoidal rule.

2) The stability function of a RK method of order p satisfies

$$R(z) = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \cdots + O(z^{p+1}) \quad \text{as } z \to 0.$$

3) Not all implicit methods are A-stable, take e.g. the θ-method:

$$y_{n+1} = y_n + (1-\theta)hf(t_n, y_n) + \theta hf(t_{n+1}, y_{n+1})$$

is A-stable for $\theta \in [\frac{1}{2}, 1]$.

($\theta = 0$: Explicit Euler, $\theta = \frac{1}{2}$: Implicit trapezoidal rule, $\theta = 1$: Implicit Euler)