ODEs BIO/CHE/PHYS

$y : I \to \mathbb{R}^s$ $\quad I = [0, T_f]$
$\subseteq \mathbb{R}^+$ $\quad (I = [0, +\infty))$

$y(t)$

$$\boxed{\frac{d}{dt} y(t) = F(t, y(t))}$$

$F : I \times \mathbb{R}^s \to \mathbb{R}^s$

KNOWN $\quad$ F CONTINUOUS

IVP

$$\begin{cases} y'(t) = F(t, y(t)) = F(y(t)) \\ y(t_0) = y_0 \end{cases}$$

$$y^{(p)}(t) = \frac{d^p y(t)}{dt^p} = f(t, y, y', \dots, y^{(p-1)})$$

$$\begin{cases} y' = z_1 \\ z_1' = z_2 \\ z_2' = z_3 \\ \dots \\ z_p' = f(t, y, z_1, \dots z_{p-1}) \end{cases} \qquad \underline{Y} = \begin{pmatrix} y \\ z_1 \\ \vdots \\ z_p \end{pmatrix}$$

$$\underline{Y}' = F(\underline{Y})$$

$$\frac{d}{dt} y(t) = F(t, y(t)) \qquad (1)$$

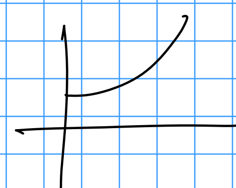
$$y(t) = y(0) + \int_0^t F(s, y(s))\,ds \qquad (2)$$

(1) + y DIFF $\iff$ (2) + F is continuous

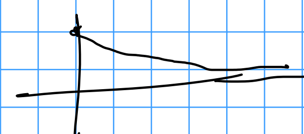
EXAMPLE DAHLQUIST'S EQUATION

$$\begin{cases} y' = -\lambda y \\ y(0) = y_0 \end{cases} \qquad \lambda \in \mathbb{R} \qquad y : I \to \mathbb{R}$$

$y = e^{-\lambda t} \cdot y_0$ $\qquad \lambda < 0$



$y_0 = 1$ $\qquad \lambda > 0$



LINEAR PROD - DEST

$$\begin{cases} c_1' = c_2 - 5c_1 \\ c_2' = 5c_1 - c_2 \end{cases} \qquad c_1' + c_2' = 0$$

$$\underline{c}' = A\,\underline{c} \qquad A = \begin{bmatrix} -5 & 1 \\ 5 & -1 \end{bmatrix}$$

$\underline{c}_0$

$$\underline{c}(t) = \underline{c}_0 + \underbrace{e^{At}}\cdot\underline{c}_0$$

$$V^T A V = D$$

$$V^T e^{At} V = e^{Dt}$$

$$e^{At} = \sum_{k=0}^{\infty} \frac{A^k t^k}{k!}$$

$$A^2 = -6A$$

$$c(t) = \underline{c}_0 + \frac{1 - e^{-6t}}{6} A\,\underline{c}_0$$

$$x' = \alpha x - \beta x y \qquad \begin{pmatrix} x \\ y \end{pmatrix}' = F\begin{pmatrix} x \\ y \end{pmatrix}$$
$$y' = \delta x y - \gamma y$$

$$\eta(x,y) = \delta x - \gamma \log(x) + \beta y - \alpha \log(y)$$

$$\frac{d}{dt}\eta(x(t), y(t)) = 0$$

$$= (\nabla \eta) \cdot \begin{pmatrix} x'(t) \\ y'(t) \end{pmatrix} = \left\langle \nabla\eta, \begin{pmatrix} x' \\ y' \end{pmatrix} \right\rangle = \underbrace{\boxed{\langle \nabla \eta, F \rangle}}_{=0}$$

$$\nabla \eta = \begin{pmatrix} \delta - \frac{\gamma}{x} \\ \beta - \frac{\alpha}{y} \end{pmatrix} \qquad F\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \alpha x - \beta x y \\ \delta x y - \gamma y \end{pmatrix}$$

$$\langle \nabla \eta, F \rangle = \delta \alpha x - \delta \beta x y - \alpha y + \gamma \beta y + \beta \delta x y$$
$$- \beta \gamma y - \alpha \delta x + \alpha \gamma = 0$$

$$\begin{cases} u' = -\dfrac{v}{r} - \alpha u \\ v' = \dfrac{u}{r} - \alpha v \end{cases} \qquad r = \sqrt{u^2+v^2}$$

$$\frac{d}{dt}\left(\frac{r^2}{2}\right) = 0 = \frac{d}{dt}\left(\frac{u^2+v^2}{2}\right) = u\frac{d}{dt}u + v\frac{dv}{dt}$$

1) $$\left[= u\left(-\frac{v}{r}\right) + v\left(\frac{u}{r}\right) = \frac{-uv + uv}{r} = 0\right.$$

2) DAMPED $$\left[= u\left(-\frac{v}{r} - \alpha u\right) + v\left(\frac{u}{r} - \alpha v\right) = -\alpha\left(u^2+v^2\right) = -2\alpha\,\frac{r^2}{2}\right.$$

$$\mathcal{E} = \frac{r^2}{2} \qquad \frac{d}{dt}(\mathcal{E}) = -2\alpha\,\mathcal{E}$$

$$\mathcal{E} = e^{-2\alpha t}\,\mathcal{E}_0$$

$$\begin{cases} u' = v \\ v' = -\sin(u) \end{cases} \qquad F = \begin{pmatrix} v \\ -\sin(u) \end{pmatrix}$$

$$\eta(t) = \frac{1}{2} v^2 - \cos(u) \qquad \nabla\eta = \begin{pmatrix} \sin(u) \\ v \end{pmatrix}$$

$$\frac{d}{dt}\eta(t) = \langle \nabla\eta, F \rangle = \sin(u)\cdot v - \sin(u)\cdot v = 0$$

$$y' = F(t,y) \quad \Rightarrow \left\{ \underbrace{y(t^n)}_{\substack{y(t^n) \\ \text{exact}}} \right\}_{n=0}^{N} \approx \left\{ y^n \right\}_{n=0}^{N}$$

$$\underbrace{y^n}_{\text{approx}} \approx y(t^n)$$

$$0 = t^0 < t^1 < \dots < t^N = T$$

$$y^{n+1} = y^n + \int_{t^n}^{t^{n+1}} F(t, y(t))\,dt = y^n + (t^{n+1} - t^n)\cdot F(t^n, y^n)$$

$$\frac{y^{n+1} - y^n}{\Delta t} = F(t^n, y(t^n))$$

$$e_{n+1} = y(t^{n+1}) - y^{n+1} =$$

$$= y(t^n) + \int_{t^n}^{t^{n+1}} y'(t)\,dt - y^n - \int_{t^n}^{t^{n+1}} F(y^n)\,dt$$

$$= \underbrace{y(t^n) - y^n}_{e_n} + \int_{t^n}^{t^{n+1}} F(t, y(t)) - F(y^n)\,dt$$

$$= e_n + \int_{t^n}^{t^{n+1}} F(t, y(t)) - F(t^n, y(t^n))\,dt$$

$$+ \int_{t^n}^{t^{n+1}} F(t^n, y(t^n)) - F(t^n, y^n)\,dt$$

$$= e_n + \underbrace{\int_{t^n}^{t^{n+1}} y'(t) - y'(t^n)}_{\varepsilon_n} + \Delta t\, F(t^n, y(t^n)) - F(t^n, y^n)$$

$$|e_{n+1}| \leq |e_n| + |\varepsilon_n| + \Delta t\, L\, \overbrace{|y(t^n) - y^n|}^{|e_n|}$$

$$\leq (1 + L\Delta t)|e_n| + |\varepsilon_n|$$

$y'(t) = M\, y(t) \qquad M \in \mathbb{R}^{s\times s} \qquad y : I \to \mathbb{R}^s$

$$y^{n+1} = y^n + \Delta t\, M y^n = \underbrace{(I + \Delta t\, M)}\, y^n$$

$$= \underbrace{(I + \Delta t\, M)^n}\, y^0$$

$$\hat{M} = S^{-1} M S \qquad \hat{M} = \begin{bmatrix} \ddots & 0 \\ 0 & \ddots \end{bmatrix} \qquad \hat{M} = \begin{bmatrix} \vdots & & 0 \\ & \boxed{\ } & \\ 0 & & \boxed{\ } \end{bmatrix}$$

$$\boxed{\hat{y}_1^{n+1} = \hat{y}_1^n + \Delta t\, \hat{M}_{11} \hat{y}_1^n} + \underbrace{\Delta t\, \hat{M}_{12} \hat{y}_2}$$

$$\Rightarrow \boxed{\hat{y}_2^{n+1} = \hat{y}_2 + \Delta t\, \hat{M}_{22} \hat{y}_2} \qquad \hat{y} = S^{-1} y$$

$$\Rightarrow \boxed{y^{n+1} = y^n + \Delta t\, q\, y^n} \qquad y'(t) = q\, y(t)$$

$$y(t) = e^{qt} y_0 \qquad y^{n+1} = (1 + \Delta t\, q)\, y^n$$

$$= (1 + \Delta t\, q)^n y_0$$

IF $\underline{q < 0}$ $\quad |y(t)| \leq |y_0|$ $\quad q \in \mathbb{C}$

IF $\mathrm{Re}(q) \leq 0$ $\quad |y(t)| < |y_0|$

$$y^{n+1} = (1+\Delta t q)\, y^n$$

$$|1+\Delta t q| \leq 1 \qquad z = \Delta t q$$

$$R(z) := 1 + z$$

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

$z \in S \iff \Delta t q \in S$ $\quad$ Δt CAN BE MODIFIED

$\Delta t \gg 0 \Rightarrow \Delta t q \notin S$ $\quad$ $\Delta t \ll 1 \Rightarrow \Delta t q \in S$

$$u'' = -u$$

$$\|F(\underline{u}) - F(\underline{v})\| \leq \| \alpha \ldots \|$$

$$u' = v$$

$$v' = -u$$

$$\underline{u}' = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \underline{u}$$

$$\lambda_{1/2} = \pm i$$

STABILITY

$$y' = q y \qquad Re(q) < 0$$

$$y^{n+1} = y^n + \Delta t \, q \, y^{n+1}$$

$$y^{n+1}(1 - \Delta t q) = y^n$$

$$y^{n+1} = \frac{y^n}{1 - \Delta t q} = \frac{y^0}{(1 - \Delta t q)^{n+1}}$$

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

TVD EXP. EULER

$$U_j^{n+1} = U_j^n + \Delta t\left[C_{j+\frac{1}{2}}\left(U_{j+1}^n - U_j^n\right) - D_{j-\frac{1}{2}}\left(U_j^n - U_{j-1}^n\right)\right]$$

$$C_{j+\frac{1}{2}},\ D_{j+\frac{1}{2}} \geq 0 \qquad \left[C_{j+\frac{1}{2}} + D_{j+\frac{1}{2}}\right]\Delta t \leq 1 .$$

IMPL. EULER

$$U_j^{n+1} = U_j^n + \Delta t\left[C_{j+\frac{1}{2}}\left(U_{j+1}^{n+1} - U_j^{n+1}\right) - D_{j-\frac{1}{2}}\left(U_j^{n+1} - U_{j-1}^{n+1}\right)\right]$$

$$\begin{aligned} U_{j+1}^{n+1} - U_j^{n+1} = {} & \left(U_{j+1}^n - U_j^n\right) + \Delta t\, C_{j+\frac{3}{2}}\left(U_{j+2}^{n+1} - U_{j+1}^{n+1}\right) \\ & - \Delta t\, C_{j+\frac{1}{2}}\left(U_{j+1}^{n+1} - U_j^{n+1}\right) - \Delta t\, D_{j+\frac{1}{2}}\left(U_{j+1}^{n+1} - U_j^{n+1}\right) \\ & + \Delta t\, D_{j-\frac{1}{2}}\left(U_j^{n+1} - U_{j-1}^{n+1}\right) \end{aligned}$$

$$\overbrace{\sum_j \left(U_{j+1}^{n+1} - U_j^{n+1}\right)}^{TV(U^{n+1})} \left(1 + \overbrace{\cancel{\Delta t\, C_{j+\frac{1}{2}} + \Delta t\, D_{j+\frac{1}{2}}}}\right)$$

$$= \underbrace{\sum_j \left(U_{j+1}^n - U_j^n\right)}_{TV(U^n)} + \Delta t \underbrace{\cancel{\sum_j \left(U_{j+2}^{n+1} - U_{j+1}^{n+1}\right) C_{j+\frac{3}{2}}}} +$$

$$\cancel{\underbrace{+\Delta t \sum_j D_{j-\frac{1}{2}}\left(U_j^{n+1}-U_{j-1}^{n+1}\right)}}$$

$$TV(U^{n+1}) \le TV(U^n)$$

$$y' = My$$

$$\boxed{y^{n+1} = y^n + \Delta t M y^{n+1}}$$

$$\underbrace{(I-\Delta t M)}_{A} \underline{y^{n+1}} = \underline{\underline{y^n}}$$

$$e_N^{FE} \approx e_N^{IG} \approx C\,\Delta t^{1}$$

$$e_{\Delta t} \approx c\,\Delta t^{p}$$

$$\underbrace{\log(e_{\Delta t})} = \log(c\,\Delta t^{p}) = \log(c) + p\,\underbrace{\log(\Delta t)}$$

$\Downarrow$ p slope

$\Downarrow$

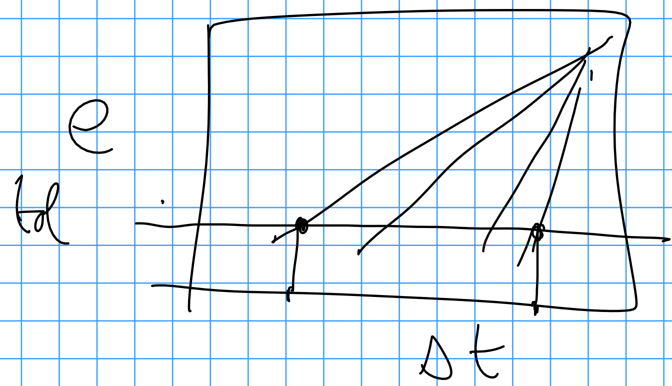
PLOT LOG-LOG error WRT Δt

$\Rightarrow$

$$\underline{\underline{e_r \approx \Delta t^{p}}} \quad ; \quad \Delta t \ll 1$$

$e_{\Delta t} \approx C \Delta t^p$ p ORDER OF ACCURACY

p larger



EXPLICIT EULER $y^{n+1} = y^n + \Delta t F(t^n, y^n)$

RUNGE-KUTTA

θ - METHOD $t^* = t^n + \theta \Delta t$

$$y^* = y^n + \theta \Delta t \, F(t^n, y^n)$$

$$y^{n+1} = y^n + \Delta t \left(\frac{2\theta - 1}{2\theta} F(t^n, y^n) + \frac{1}{2\theta} F(t^*, y^*) \right)$$

HIGH ORDER?

LOCAL TRUNCATION $\Rightarrow O(\Delta t^3)$

$$y(t^{n+1}) = \underbrace{y(t^n) + \Delta t\, y'(t^n) + \frac{\Delta t^2}{2} y''(t^n) + O(\Delta t^3)}$$

$$y(t^*) = y(t^n) + \Delta t\,\theta\, y'(t^n) + O(\Delta t^2)$$

$$y^* - y(t^*) = \underbrace{-y(t^n) + y^n} - \Delta t\,\theta \underbrace{y'(t^n)} + \Delta t\,\theta\, F(\underbrace{t^n, y^n}) + O(\Delta t^2)$$

$\Rightarrow$ SUPPOSING $y^n = y(t^n)$

$$y^* = y(t^*) + O(\Delta t^2)$$

$$y^{n+1} = y(t^n) + \Delta t\left[\frac{2\theta - 1}{2\theta} F(y^n, t^n) + \frac{1}{2\theta} F(t^*, y^*)\right]$$

SUPPOSE $F(t, y) = F(y)$

$$= y(t^n) + \Delta t\left[\frac{2\theta-1}{2\theta} F(y^n) + \frac{1}{2\theta}\left[F(y^n) + \Delta t\,\theta \frac{d F(y)}{dt} + O(\Delta t^2)\right]\right]$$

$$= y(t^n) + \Delta t \left[F(y^n) + \frac{\Delta t \cancel{\theta}}{2 \cancel{\theta}} \frac{d}{dt}(y') \right] + O(\Delta t^3)$$

$$= y(t^n) + \Delta t \, y'(t^n) + \frac{\Delta t^2}{2} y''(t^n) + O(\Delta t^3)$$

RK METHOD $\quad S$ stages

$A \in \mathbb{R}^{S \times S} \quad b, c \in \mathbb{R}^S \quad y^n$ KNOWN

? y^{n+1}

$$y^{(k)} = y^n + \Delta t \sum_{j=1}^{S} a_{kj} F(t^n + c_j \Delta t, y^{(j)}) \quad \forall k = 1, \dots, S$$

$$y^{n+1} = y^n + \Delta t \sum_{j=1}^{S} b_j F(t^n + c_j \Delta t, y^{(j)})$$

EXPLICIT RK IF $a_{kj} = 0 \quad \forall j \geq k$

A IS STRICTLY LOW TRIANGULAR

$y^{(1)} = y^n$

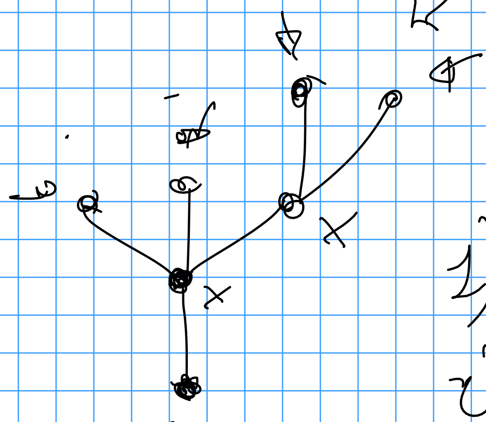
$$y^{(2)} = y^n + \underbrace{\theta}_{a_{21}} \Delta t \, F(y^{(1)}, t^n + \Delta t \underbrace{\theta}_{c_1})$$

$$y^{n+1} = y^n + \Delta t\left[\underbrace{\frac{2\theta-1}{2\theta}}_{b_1} F(y^{(1)}) + \underbrace{\frac{1}{2\theta}}_{b_2} F(y^{(2)})\right]$$

$$\boxed{\begin{array}{c|c} c & A \\ \hline & b^T \end{array}}$$

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \theta & \theta & 0 \\ \hline & \frac{2\theta-1}{2\theta} & \frac{1}{2\theta} \end{array} \Longrightarrow \begin{array}{c|cc} 0 & & \\ \theta & \theta & \\ \hline & \frac{2\theta-1}{2\theta} & \frac{1}{2\theta} \end{array}$$

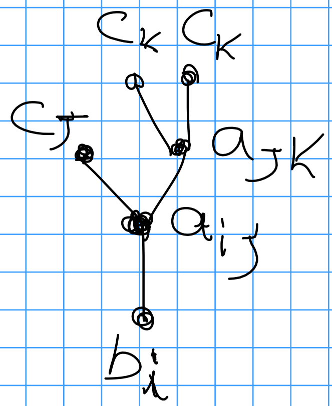
$$\sum_k A_{ik} = c_i$$



$= \tau$ TREE

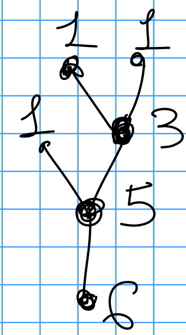
1) ORDER τ = # NODES

2) $\Phi_\tau(a_{ij}, b_i, c)$



2) $\Phi_\tau := \sum_{i,j,k} b_i a_{ij} a_{jk} c_j c_k^2$

3) γ_τ



$\gamma_\tau = 6 \cdot 5 \cdot 3 \cdot 1 \cdot 1 = 15 \cdot 6 = 90$

1) order

2) $\Phi(A, b, c)$

3) γ

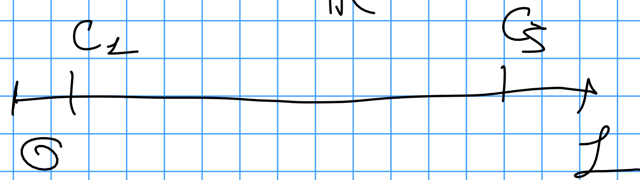
RK scheme is of order p

$\forall \; d \leq p$

$\forall \; \tau$ of order d

$\Phi_\tau(A, b, c) = \frac{1}{\gamma_\tau}$

$$\int_{t^n}^{t^{n+1}} f(t)\,dt \approx \sum_{i=1}^{s} \underset{\mathbb{R}}{\underset{\uparrow}{w_i}}\, f(t^n + \underline{c_i}\,\Delta t)$$



$$0 \le c_1 < \dots < c_j < \dots < c_s \le 1$$

φ_i LAGRANGIAN INTERP. POLY

$$\varphi_i(t^n + c_j \Delta t) = \delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

$$\underline{\underline{y^{(j)}}} \approx y(t^n + c_j \Delta t) = \int_{t^n}^{t^n + c_j \Delta t} F(s, y(s))\,ds$$

$$y^{(j)} \approx y^n + \underbrace{\int_{t^n}^{t^n + c_j \Delta t} \sum_i \varphi_i(x)}_{a_{ji} := \int_{t^n}^{t^n + c_j \Delta t} \varphi_i(x)\,dx} \cdot \underbrace{F(t^n + c_i \Delta t, y^{(i)})}_{F^{(i)}}$$

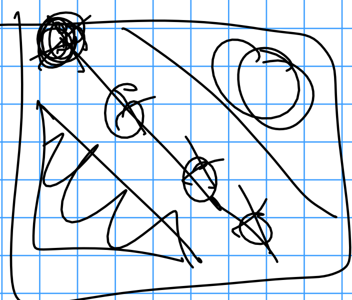
$$y^{(j)} = y^n + \Delta t \sum \tilde{a}_{ji}\, F^{(i)}$$

GAUSS-LEGENDRE   S STAGES → QUAD POINTS

$$f \simeq \sum_i b_i f(c_i) + O(\Delta t^{2S+1}) \Rightarrow \boxed{2S}$$

$$\{c_i\} \subseteq (0,1)$$

GAUSS-LOBATTO   S stages   2S $\Rightarrow$ $\boxed{2S-1}$

A  $\Rightarrow$ D. IMPLICIT

$$\boxed{y' = qy}$$

$Re(q) \le 0$ $R(z)$ $z = \Delta t q$

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

$\Delta t \sum a_{ij} q Y^{(j)}$

$$Y \in \mathbb{R}^{STAGES}$$

$$Y = \mathbb{1} y^n + \Delta t q A Y$$

$$\mathbb{1} = \begin{pmatrix}1\\ \vdots\\ 1\end{pmatrix} \in \mathbb{R}^{STAGES}$$

$$y^{n+1} = y^n + \Delta t\, q\, b^T \bar{Y} = y^n + \Delta t\, q\, b^T (I - \Delta t\, q A)^{-1} \mathbb{1} y^n$$

$$(I - \Delta t\, q\, A)\bar{Y} = \mathbb{1} y^n$$

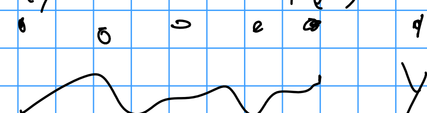
$$\bar{Y} = (I - \Delta t\, q A)^{-1} \mathbb{1} y^n$$

$$= \Big(\underbrace{1}_{\in \mathbb{R}} + z\, \underbrace{b^T (I - zA)^{-1} \mathbb{1}}_{\in \mathbb{R}}\Big) y^n$$

$$y^{n+1} = \underline{\underline{R(z)}}\, y^n \qquad R(z) = \frac{NUM(z)}{DEN(z)}$$

A-B

$F(y^{n+1-k})$ $\quad F(y^n)$



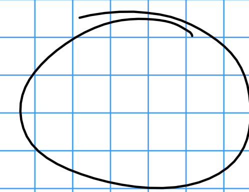
y^{n+1}

$F(y^{n+1}) \to ?$

A-M

y^{n+1}

RELAXATION



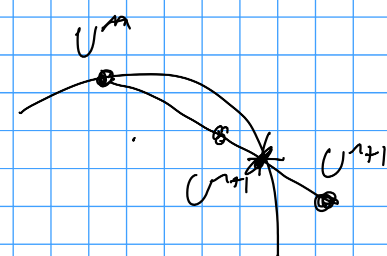
$u' = F(u)$

$$\frac{\langle u, u\rangle}{2} = \sum_{i=1}^{m} \frac{u_i^2}{2}$$

$$\frac{1}{2}\frac{d\langle u, u\rangle}{dt} = 0 \iff \frac{\cancel{2}}{\cancel{2}}\left\langle u, \frac{du}{dt}\right\rangle = \langle u, F(u)\rangle = 0$$

≤ 0

$$\Rightarrow \frac{d}{dt}\mathcal{E}(u) \leq 0 \qquad \mathcal{E}(u) = \frac{\langle u, u\rangle}{2}$$



$$U^{n+1} = U^n + \Delta t \sum_{j=1}^{s} b_j F(U^{(j)})$$

$\mathbb{R} \ni \gamma \simeq 1$

$$U_\gamma^{n+1} = U^n + \gamma \underbrace{\Delta t \sum_{j=1}^{s} b_j F(U^{(j)})}_{\Delta U} = U^n + \gamma \underline{\Delta U}$$

$$\langle U_\gamma^{n+1}, U_\gamma^{n+1}\rangle \overset{!}{=} \langle U^n, U^n\rangle$$

$$\langle U^n + \gamma \Delta U, U^n + \gamma \Delta U\rangle \overset{!}{=} \langle U^n, U^n\rangle$$

$$\cancel{\langle U^n, U^n\rangle} + 2\gamma \langle U^n, \Delta U\rangle + \gamma^2 \langle \Delta U, \Delta U\rangle \overset{!}{=} \cancel{\langle U^n, U^n\rangle}$$

$\gamma = 1 \qquad \gamma \neq 0$

$$\gamma = \frac{-2\langle U^n, \Delta U\rangle}{\langle \Delta U, \Delta U\rangle}$$

$$\begin{cases} U_\gamma^{n+1} := U^n + \gamma \Delta U \\ t_\gamma^{n+1} := t^n + \gamma \Delta t \end{cases}$$

$\Rightarrow$ RK METHOD SAME ORDER OF ACCURACY

VERIFY $\frac{d\mathcal{E}}{dt} = 0$

$$\langle U_\gamma^{n+1}, U_\gamma^{n+1}\rangle = \langle U^n, U^n\rangle + 2\gamma \langle U^n, \Delta U\rangle + \gamma^2 \langle \Delta U, \Delta U\rangle$$

$$= \langle U^n, U^n\rangle + 2\gamma \Delta t \sum_{j=1}^{s} b_j \langle U^n, F(U^{(j)})\rangle + \gamma^2 \langle \Delta U, \Delta U\rangle$$

≈ 0

≤ 0

$$+ 2\gamma \Delta t \sum_j b_j \langle U^{(j)}, F(U^{(j)})\rangle \underbrace{- 2\gamma \Delta t \sum_j b_j \langle U^{(j)}, F(U^{(j)})\rangle}_{=0}$$

$= 0$ (CONSERV)

≤ 0 (DISSIPATIVE)

$$\langle U_\gamma^{n+1}, U_\gamma^{n+1} \rangle = \langle U^n, U^n \rangle + 2\gamma \Delta t \sum_j b_j \langle U^{(j)}, F(U^{(j)}) \rangle \Big] \text{ OK}$$

$$\underbrace{+ 2\gamma \Delta t \sum_j b_j \langle U^n - U^{(j)}, F(U^{(j)}) \rangle + \gamma^2 \langle \Delta U, \Delta u \rangle}_{\overset{!}{=} 0}$$

SCALAR EQUATION FOR γ

$$\gamma = \frac{2 \Delta t \sum_j b_j \langle U^{(j)} - U^n, F(U^{(j)}) \rangle}{\langle \Delta U, \Delta u \rangle} \qquad \gamma = 1 + O(\Delta t^{p-1})$$

$\langle U_\gamma^{n+1}, U_\gamma^{n+1} \rangle = \langle U^n, U^n \rangle$ IF $\langle U, F \rangle = 0$

$\langle U_\gamma^{n+1}, U_\gamma^{n+1} \rangle \leq \langle U^n, U^n \rangle$ IF $\langle U, F \rangle \leq 0$

BE CAREFULL ! EXPLICIT EULER $A_{12} = 0$

$U^{(1)} = U^n$

$U^{n+1} = U^n + \Delta t F(U^{(1)})$

$U^{(1)} = U^n$

$$\underline{U^{(1)} = U^n}$$

$$\gamma = \frac{2\Delta t \langle \overbrace{U^{(1)} - U^n}^{=0}, F(U^{(1)}) \rangle}{\langle \Delta U, \Delta U \rangle} = 0 \,!$$

np.dot(u, u)

$\eta(u)$

PENDULUM

LOTKA-VOLT

...

$\Rightarrow$ ODEs ✓

$\Rightarrow$ LYAPUNOV ✓

$\Rightarrow$ PDEs

$$V(u) : \underline{\langle F(u), V(u) \rangle} = 0 \quad (\leq) 0$$

$$\nabla_u \eta(u) = V(u)$$

$$U' = F(u)$$

$$\frac{d\eta(u)}{dt} = \langle \nabla_u \eta(u), \frac{du}{dt} \rangle = \overbrace{\langle \nabla_u \eta(u), F(u) \rangle}^{(\leq) 0 \;\; = 0}$$

$$U^{n+1}_\gamma = U^n + \gamma \Delta U$$

$$\eta(U^{n+1}_\gamma) = \eta(u^n) + \underbrace{\gamma \langle \Delta u, \overbrace{\nabla_u \eta(u^n)}^{V(U^n)} \rangle}_{} + O(\Delta t^2)$$

?

$$+\gamma \Delta t \sum_j b_j \langle F(U^j), V(U^j) \rangle \quad \begin{pmatrix} \leq 0 \\ = 0 \end{pmatrix}$$

$$-\gamma \Delta t \sum_j b_j \langle F(U^j), V(U^j) \rangle$$

$$0 \overset{!}{=} \underbrace{\eta(U^n + \gamma \Delta U)}_{\nabla} - \eta(U^n) - \gamma \Delta t \sum_J b_J \langle F(U^{(J)}), \cancel{V(U^n)} - V(U^{(J)}) \rangle$$

SOLVE FOR γ

$$\underbrace{\eta(U^n + \gamma \Delta U) = \eta(U^n) + \gamma \underbrace{\Delta t \sum_J b_J \langle V(U^{(J)}), F(U^{(J)}) \rangle}}$$

SHOULD BE VERIFIED

$$r(\gamma) = \eta(U^n + \gamma \Delta U) - \eta(U^n) - \gamma \Delta t \sum_J b_J \langle V(U^{(J)}), F(U^{(J)}) \rangle$$

$\Rightarrow$ NON LINEAR SOLVER $\rightarrow \gamma$

NEWTON METHOD

$r(\gamma) = 0$

$\partial_\gamma r(\gamma) = \langle V(U^n + \gamma \Delta U), \Delta U \rangle - \Delta t \sum \ldots$

$$c_i^{n+1} = c_i^n + \Delta t \left[\sum_j p_{ij}(c^n) - \sum d_{ij}(c^n) \cdot \frac{c_i^{n+1}}{c_i^n} \right]$$

$$\sum_i c_i^{n+1} = \sum_i c_i^n + \Delta t \left[\sum_{i,j} d_{ij}(c^n) - \underbrace{\sum d_{ij}(c^n) \frac{c_i^{n+1}}{c_i^n}}_{\neq} \right]$$

$$c_i^{n+1} = c_i^n + \Delta t \left[\underbrace{\sum_j p_{ij}(c^n) \frac{c_j^{n+1}}{c_j^n}} - \sum d_{ij}(c^n) \cdot \frac{c_i^{n+1}}{c_i^n} \right]$$

$$\sum_i c_i^{n+1} = \sum_i c_i^n + \Delta t \left[\underbrace{\sum_{i,j} d_{ij} \frac{c_i^{n+1}}{c_i^n}} - \underbrace{\sum_{i,j} d_{ij} \frac{c_i^{n+1}}{c_i^n}} \right] = \sum_i c_i^n$$

$$\Pi_{ij}(c^n) = \begin{cases} 1 + \Delta t \sum_{i=1}^{I} \dfrac{d_{ij}(c^n)}{c_i^n} > 0 & i = j \\ -\Delta t \dfrac{p_{ij}(c^n)}{c_j^n} \leq 0 & i \neq j \end{cases}$$

$$\underline{\Pi} \cdot \underline{c}^{n+1} = \underline{c}^n$$

$$M x = b \qquad b > 0 \Rightarrow x > 0$$

$$M_{ii} > 0 \qquad M_{ij} \leq 0 \quad i \neq j$$

$$\sum_{i} |M_{ij}| < |M_{ii}|$$

$$|M_{ii}| = \underbrace{1 + \Delta t \sum_{j=1}^{I} \frac{d_{ij}(c^n)}{C_i^n}}_{\geq 0} > \Delta t \sum_{j=1}^{I} \frac{d_{ij}(c^n)}{C_i^n} =$$

$$= \Delta t \sum_{j=1}^{I} \frac{p_{ji}(c^n)}{C_i} = - \sum_{\substack{j=1 \\ j \neq i}}^{I} M_{ji} = \sum_{j=1}^{I} |M_{ji}|$$

JACOBI ITERATIVE

$$M = D - L \qquad D > 0 \qquad \underline{\underline{L > 0}} \qquad D_{ii} = M_{ii}$$

$$L = -(M - D)$$

$$M x = b \qquad D x = L x + b$$

$$D x^{(k+1)} = L x^{(k)} + b \qquad A x^* = b$$

$$x^{(k+1)} = D^{-1}(L x^{(k)} + b) \qquad D x^* = L x^* + b$$

$$D^{-1} L \qquad x^* = D^{-1}(L x^* + b)$$

$$e^{(k)}{}_i = x^{(k)} - x^*$$

$$e^{(k)} = x^{(k)} - x^* = D^{-1}(L x^{(k-1)} + b) + D^{-1}(L x^* + b)$$

$$= D^{-1} L (x^{(k-1)} - x^*) = \underbrace{D^{-1} L}_{\rho(\ ) < 1} e^{(k-1)}$$

$$x^{(k+1)} = \underbrace{D^{-1}}_{\geq 0} (\underbrace{L}_{\geq 0} \underbrace{x^{(k)}}_{\geq 0} + \underbrace{b}_{\geq 0}) \geq 0$$

$$\|D^{-1} L\|_\infty = \max_i \sum_{j=1}^{I} |(D^{-1} L)_{ji}| = \max_i \sum_j \frac{|L_{ji}|}{|D_{ii}|} =$$

$$= \max_i \frac{\sum_j |L_{ji}|}{|D_{ii}|} < 1. \qquad \boxtimes$$

$\boxed{\text{ODE}}$ → THEORETICAL → $\exists!$ SOL

→ DON'T KNOW EXACT

→ APPROXIMATE

→ EXPLICIT EULER → EASY, $\Delta t < C$ ⇒ PROPERTIES POS STAB

→ CONSERVATION (MASS)

→ NOT ENERGY PRESERVING

→ IMPLICIT

→ NONLINEAR SOLVER

→ STABILITY

RUNGE-KUTTA METHODS

1 STEP $U^n \to U^{n+1}$

S STAGES

SSPRK (10, 4) → STORAGE PROB.

ARBITRARY ORD ACC

IMPLICIT → GL COLL METHOD

MULTISTEP

$\underbrace{U^{n-k+1}, \dots, U^n}$ → U^{n+1}

EXPLICIT ⇒ K STEPS → K-ORDER

EXPLICIT

DeC / ADER $\Rightarrow$ $\underbrace{\text{CONVERGE SEQ IMPLICIT RK}}$

ARBITRARY H ORDER

ITERATING PROCEDURE K = ORDER

AS RK METHODS (STAGES $\simeq$ K · M)

ORDER^2

ENTROPY / ENERGY / LIYAPUNEV FUNCTION

SCALAR CONSTRAINTS

ENFORCED

RELAXATION RUNGE-KUTTA

1) extra scalar equation $\Rightarrow \gamma$

2) $\Rightarrow$ ORDER AS THE ORIGINAL

OR BETTER

POSITIVITY SOLUTION $\Rightarrow$ PROD / DEST PROBLEMS

PATANKAR TRICK, MODIFIED P.T. $\Rightarrow$ LINEAR MASS MATRIX TO BE INVERTED

$\Rightarrow$ + , (CONSERVATION), ARBITRARY H.O.

mPRK order 3 STAGES 4

SSPRK ADDING DOF

↳ PRESERVE STABILITY TVD

(EXPLICIT EULER IS PRESERVING)

DeC

OR	STAGES
2	2
3	5
4	10