Lec 18.

Hamiltonian dynamics.

mixed implicit-explict methods.

$u_{n+1} = \Psi_h(u_n)$ order p.

modified eq.

$f_2 = f_3 = \cdots = f_p = 0$.

$$\dot{\tilde{u}} = f(\tilde{u}) + h^p f_{p+1}(\tilde{u}) + O(h^{p+1}).$$

Pf: LTE.

$$u(t_{n+1}) - \Psi_h(u(t_n)) \sim O(h^{p+1}).$$

$$\Phi_h(u(t_n)) = u(t_n) + \int_{t_n}^{t_{n+1}} \dot{\tilde{u}}(s)\,ds$$

$$= u(t_n) + \int_{t_n}^{t_{n+1}} f(\tilde{u}(s))\,ds \longrightarrow u(t_{n+1})$$

$$+ h \int_{t_n}^{t_{n+1}} \cancel{f_2(\tilde{u}(s))}\,ds + \cdots + h^{p-1} \int_{t_n}^{t_{n+1}} \cancel{f_p(\tilde{u}(s))}\,ds$$

$$+ h^p \int_{t_n}^{t_{n+1}} f_{p+1}(\tilde{u}(s))\,ds + O(h^{p+2})$$

$$= u(t_{n+1}) + O(h^{p+1})$$

$\square$.

Next show for each term

$$f_p(\tilde{u}) = J^{-1} D_u H_p(\tilde{u}).$$

We do by induction.

$P = 1$. ✓

Now assume up to p. proven.

To show $f_{p+1} = J^{-1} D H_{p+1}$

Derivative $J f_{p+1}$ is symmetric.

$$\dot{\tilde{u}} = f(\tilde{u}) + \cdots + h^{p-1} f_p(\tilde{u})$$

$$\tilde{\varphi}_{p,h}(u_0)$$

$u_1 = \Phi_h(u_0)$

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

$$u_0 \longrightarrow \tilde{\varphi}_{p,h}(u_0)$$

flow map of truncated dynamics.

$$\Phi_h(u_0) = \tilde{\varphi}_{p,h}(u_0) + h^{p+1} f_{p+1}(u_0) + O(h^{p+2})$$

$$(*)\ D_{u_0}\Psi_h(u_0) = D_{u_0}\widetilde{\varphi}_{p,h}(u_0) + h^{p+1} D_{u_0} f_{p+1}(u_0)$$

$$+ O(h^{p+2}).$$

Use symplecticity.

$$J = \left(D_{u_0}\Psi_h\right)^T J \left(D_{u_0}\Psi_h\right)$$

plugin $(*)$

$$= \underbrace{\left(D_{u_0}\widetilde{\varphi}_{p,h}\right)^T J \left(D_{u_0}\widetilde{\varphi}_{p,h}\right)}_{J \text{ (Poincaré)}}$$

$$+\Big[\big(D_{u_0}\tilde{\varphi}_{p,h}\big)^T J\, D_{u_0} f_{p+1}$$

$$+\ \big(D_{u_0} f_{p+1}\big)^T J\, D_{u_0}\tilde{\varphi}_{p,h}\Big]\cdot h^{p+1}$$

$$+\ O(h^{p+2})$$

use $D_{u_0}\tilde{\varphi} = I + O(h)$

$$J + h^{p+1}\Big[\underbrace{J\, D_{u_0} f + (D_{u_0} f)^T J}_{=0}\Big] + O(h^{p+2})$$

$\square$.

Finally. show

$$\left| H(u_n) - H(u_0) \right| \lesssim h^p$$

FOR LONG TIME.

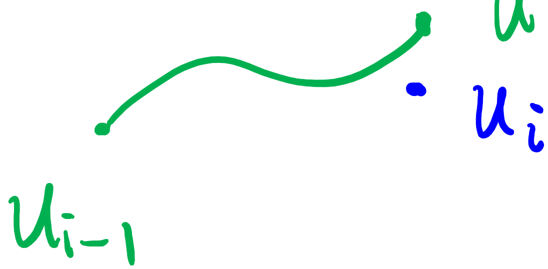
$$\begin{array}{ccccc} & H(u_n) & & H(u_0) & \\ 2 & | & & | & 3 \\ & H^{(m)}(u_n) & \underset{1}{-} & H^{(m)}(u_0) & \end{array}$$

① $$\left| H^{(m)}(u_n) - H^{(m)}(u_0) \right|$$

$$\leq \sum_{i=1}^{n} \left| H^{(m)}(u_i) - H^{(m)}(u_{i-1}) \right|$$

$$\tilde{u}_i = \tilde{\varphi}_{m,h}(u_{i-1})$$

flow



$$= \sum_{i=1}^{n} \left| H^{(m)}(u_i) - H^{(m)}\left(\tilde{\varphi}_{m,h}(u_{i-1})\right) \right|$$

$\downarrow$

globally Lipschitz

$$\le L \sum_{i=1}^{n} \left\| u_i - \tilde{\varphi}_{M,h}(u_{i-1}) \right\|$$

LTE

$$= L \sum_{i=1}^{n} h^{M+1} = L(nh)h^{M}$$

$$= L \cdot T h^{M}$$

② ③

$$H^{(M)}(u) = H(u) + h^{p} H_{p+1}(u) + O(h^{p+1})$$

$$|H(u) - H^{(M)}(u)| \lesssim h^p$$

$$|H(u_n) - H(u_0)| \lesssim \underbrace{h^p + T h^M}_{\text{balance}}$$

$$h^p \sim T h^M \Rightarrow T \sim h^{p-M}$$

T superalgebraically long.

$\longrightarrow$ also exponential rate.

$$T \sim c\, e^{\frac{\gamma}{h}}$$ $\longrightarrow$ long time.

$$\dot{u} = Lu + N(u,t)$$

$\uparrow$

linear matrix. difficult

nonlinear easy.

Implicit - explicit (IMEX)

Implicit for L

explicit " N.

Ex. Backward - Forward Euler.

$$u_{n+1} = u_n + hL\,u_{n+1} + hN(u_n, t)$$

$$u_{n+1} = (I - hL)^{-1}\left(u_n + hN(u_n, t)\right)$$

RAS. L is scalar.

$$\mathcal{N}(u_n) = N u_n$$

$$z = Lh, \quad w = Nh$$

$$u_{n+1} = (1-z)^{-1}(1+w)\,u_n$$

$$\Rightarrow \left|\frac{1+w}{1-z}\right| \le 1 \Rightarrow |1+w| \le |1-z|$$

$$|z| \gg 1, \quad |1+w| \lesssim |z|$$

also consider $|z| \sim O(1)$

① $z = 1$. u_{n+1} cancelled. (coincidence)

② $z < 0 \Rightarrow |1+w| \sim O(1)$

Generalization:

① $AM_n - AB_m$ scheme.

② Mixed w. RK.

Exponential time-differencing (ETD)

Duhamel's principle.

$$u(t_{n+1}) = e^{Lh} u(t_n) + \underbrace{\int_{t_n}^{t_{n+1}} e^{L(t_{n+1}-s)} N(u(s), s)\, ds}_{\text{Quadrature.}}$$

ETD-ABn.

(exer) RAS for ETD-AB1.

Compute

$$e^{A} u$$

Apply matrix exp. to a vector.

① Taylor expansion

$$e^{x} = \sum_{n=0}^{\infty} \frac{1}{n!} x^{n}$$

$$e^{A} = \sum_{n=0}^{\infty} \frac{1}{n!} A^{n}$$

$$e^{A} u \approx \sum_{n=0}^{N} \frac{1}{n!} A^{n} u$$

Try other expansion.

e.g. $\|A\|_2 \le 1$. A Hermitian

Chebyshev expansion.

$$e^A u \approx \sum_{n=0}^{N} c_n T_n(A) u$$

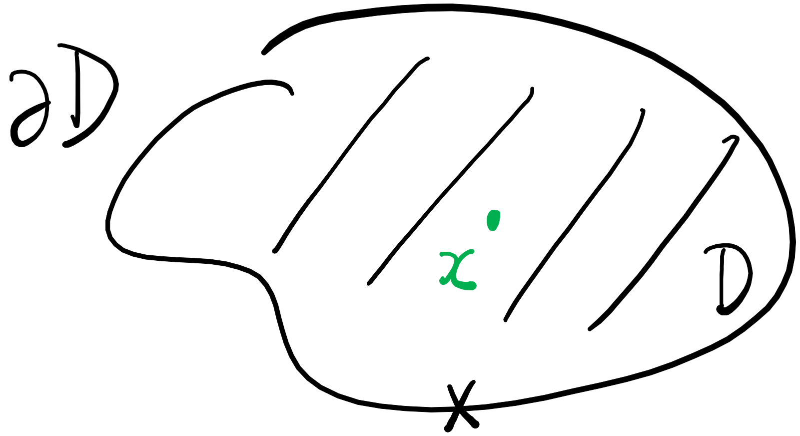
Chebyshev poly. (of 1st kind)

② Diagonalization.

$$A = VDV^{-1}, \quad D \text{ diagonal}.$$

$$e^{A} = V e^{D} V^{-1}$$

③ Contour integral.



$f(z)$ analytic.

$$f(x) = \frac{1}{2\pi i} \oint_{\partial D} \frac{f(z)}{z - x}\, dz$$

Cauchy contour integral formula.