Lec 16.

Hamiltonian system.

$$H : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}$$

$\uparrow$ momentum $\quad$ $\uparrow$ space.

$p \quad q$

$$\begin{cases} \dot{p} = -\dfrac{\partial H(p,q)}{\partial q} \\ \dot{q} = \dfrac{\partial H(p,q)}{\partial p} \end{cases}$$

$$H(p,q) = T(p) + V(q) \qquad \text{separable}$$

Ex. N - particles interacting in a potential field $V(q_1, \cdots, q_N)$

$$H(p,q) = \sum_{i=1}^{N} \frac{1}{2m_i} p_i^2 + V(q_1, \cdots, q_N)$$

$$\begin{pmatrix} \dot{p}(t) \\ \dot{q}(t) \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & -I_d \\ I_d & 0 \end{pmatrix}}_{J^{-1}} \begin{pmatrix} \dfrac{\partial H(p(t), q(t))}{\partial p} \\ \dfrac{\partial H(p(t), q(t))}{\partial q} \end{pmatrix} \to \nabla_u H(u(t))$$

$$\varphi_t(p_0, q_0) = (p(t), q(t)) := u(t)$$

$$\boxed{\frac{du(t)}{dt} = J^{-1} \nabla_u H(u(t))}$$

$$J = \begin{bmatrix} 0 & I_d \\ -I_d & 0 \end{bmatrix} \qquad \boxed{J^{-1} = -J = J^T}$$

Area preserving $\Rightarrow$ Consider

Jacobian

$$\Phi_t(p_0, q_0) = \begin{bmatrix} \frac{\partial p(t)}{\partial p_0} & \frac{\partial q(t)}{\partial p_0} \\ \frac{\partial p(t)}{\partial q_0} & \frac{\partial q(t)}{\partial q_0} \end{bmatrix}$$

$$\Phi_t(u_0) = \frac{\partial u(t)}{\partial u_0}$$

Want to show: $\left| \Phi_t(u_0) \right| = 1$.

Thm (Poincaré) Hamiltonian dynamics

$$\Phi_t^T J \, \Phi_t = J$$

symplectic

$u(t) = \varphi_t(u_0)$

Symplectic $\Rightarrow$ area preserving

$$\det\left(\Phi_t^T J \, \Phi_t\right) = \det(\Phi_t)^2 \cancel{\det(J)} = \cancel{\det(J)}$$

$$\Rightarrow \det(\Phi_t) = \pm 1. \quad \text{for all } t.$$

$$\det \Phi_t = \det \Phi_0 = 1 \quad (\text{continuity})$$

Pf: $\Phi_0 = I \qquad \Phi_0^T J \Phi_0 = J. \quad t=0$ ✓

$$\frac{d}{dt}\Phi_t = \frac{d}{dt}\nabla_{u_0}\varphi_t(u_0) = \nabla_{u_0}\frac{d}{dt}\varphi_t(u_0)$$

$$= \nabla_{u_0}\left(J^{-1}\nabla_u H(\varphi_t(u_0))\right)$$

$$= J^{-1}\underbrace{\nabla_u^2 H(u(t))}_{\text{Hessian. symmetric}} \cdot \Phi_t$$

$$\frac{d}{dt}\left(\Phi_t^T J \Phi_t\right)$$

$$= \Phi_t^T \nabla_u^2 H \left(-J^{-1}\right) J \Phi_t$$

$$+ \Phi_t^T J J^{-1} \nabla_u^2 H \Phi_t = 0 \quad \square.$$

Symplectic scheme.

Discrete flow map

$$\varphi_n : u_0 \mapsto u_n(u_0)$$

Jacobian $\Phi_n := \dfrac{\partial \varphi_n(u_0)}{\partial u_0}$

$$\Phi_n^T J \Phi_n = J$$

Lemma: $f : \mathbb{R}^n \to \mathbb{R}^n$. $f \in C^1(\mathbb{R}^n)$

$Df(u)$ is symmetric i.e.

$$\frac{\partial f_i}{\partial u_j} = \frac{\partial f_j}{\partial u_i}$$

Then $\exists$ $H : \mathbb{R}^n \longrightarrow \mathbb{R}$.

s.t. $f(u) = D_u H(u)$.

Pf: $H(u) = \int_0^1 u \cdot f(tu)\, dt$

$$\frac{\partial H(u)}{\partial u_j} = \int_0^1 f_j(tu)\, dt$$

$$+ \int_0^1 \sum_{i=1}^{N} u_i \frac{\partial f_i(tu)}{\partial u_j} \cdot t\, dt$$

$$= \int_0^1 f_j(tu) + \sum_{i=1}^{N} u_i \cdot \frac{\partial f_j(tu)}{\partial u_i}\, t\, dt$$

$$= \int_0^1 \frac{d}{dt}\left(t\, f_j(tu)\right) dt$$

$$= f_j(u) \qquad \square.$$

<u>Thm</u>. (Inverse of Poincaré)

$f : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$. $f \in C^1(\mathbb{R}^{2d})$

flow map of $\dot{u} = f(u)$

is symplectic. Then $\exists$ H

$$f = J^{-1} D_u H.$$

Pf: Only need to show the derivative of Jf is symmetric.

$$\dot{u} = f(u) \qquad \Phi_t = \frac{\partial u(t)}{\partial u_0}$$

$$\dot{\Phi} = D_u f(u)\, \Phi$$

$$\Phi_t^T J \Phi_t = J$$

$$\Rightarrow \left(\frac{d}{dt}\Phi_t\right)^T J \Phi_t + \Phi_t^T J \frac{d\Phi_t}{dt} = 0$$

$$\Rightarrow \Phi_t^T (D_u f)^T J \Phi_t + \Phi_t^T J (D_u f) \Phi_t = 0$$

$$\Rightarrow \Phi_t^T \left(\underbrace{(J D_u f) - (J D_u f)^T} \right) \Phi_t = 0$$

Φ_t arbitrary. $\Rightarrow$ $= 0$.

$\Rightarrow \quad J D_u f$ symmetric

$$\Rightarrow \quad f = J^{-1} D_u H \qquad \square$$

$$\varphi : \mathbb{R}^d \to \mathbb{R}^d . \qquad V \subset \mathbb{R}^d$$

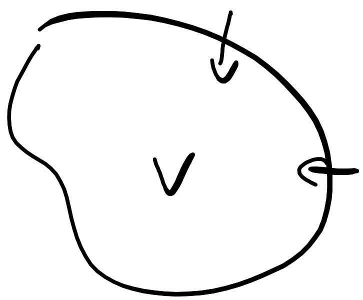
$$\mathrm{vol}(V) = \int_V d\vec{x}$$

$$\mathrm{vol}(\varphi(V)) = \int_{\varphi(V)} d\varphi(\vec{x}) = \int_V \underbrace{\left|\det \frac{\partial \varphi}{\partial x}\right|}_{\shortparallel} d\vec{x}$$

$$\Phi_t^T J \Phi_t = J \Rightarrow \det \Phi_t = \pm 1.$$

$\det \Phi_t$ is continuous w.r.t. t

$$\det \Phi_0 = 1.$$



volume preserving.

$$\nabla \cdot \varphi = \sum_{i=1}^{d} \frac{\partial}{\partial x_i} \varphi_i = 0.$$

$$\dot{u} = f(u) = J^{-1} D_u H(u) = \begin{bmatrix} -D_q H \\ D_p H \end{bmatrix}$$

$$D_p \cdot (-D_q H) + D_q \cdot (D_p H) = 0 .$$

$\Rightarrow$ volume preserving.

Symplectic scheme.

$$u_{n+1} = \Phi_h (u_n)$$

$$\Phi_n = \frac{\partial u_n}{\partial u_0}. \qquad \Phi_n^T J \Phi_n = J.$$

Need to show

$$\underbrace{\Phi_{n+1}^T J \Phi_{n+1} = \Phi_n^T J \Phi_n} = \cdots = J$$

Examples of symplectic schemes.

Symplectic Euler. (1)

implicit

$$\begin{cases} p_{n+1} = p_n - h D_q H(p_{n+1}, q_n) \\ q_{n+1} = q_n + h D_p H(p_{n+1}, q_n) \end{cases}$$

$$H(p, q) = T(p) + V(q)$$

$$\begin{cases} p_{n+1} = p_n - h D_q V(q_n) \\ q_{n+1} = q_n + h D_p T(p_{n+1}) \end{cases}$$

explicit!

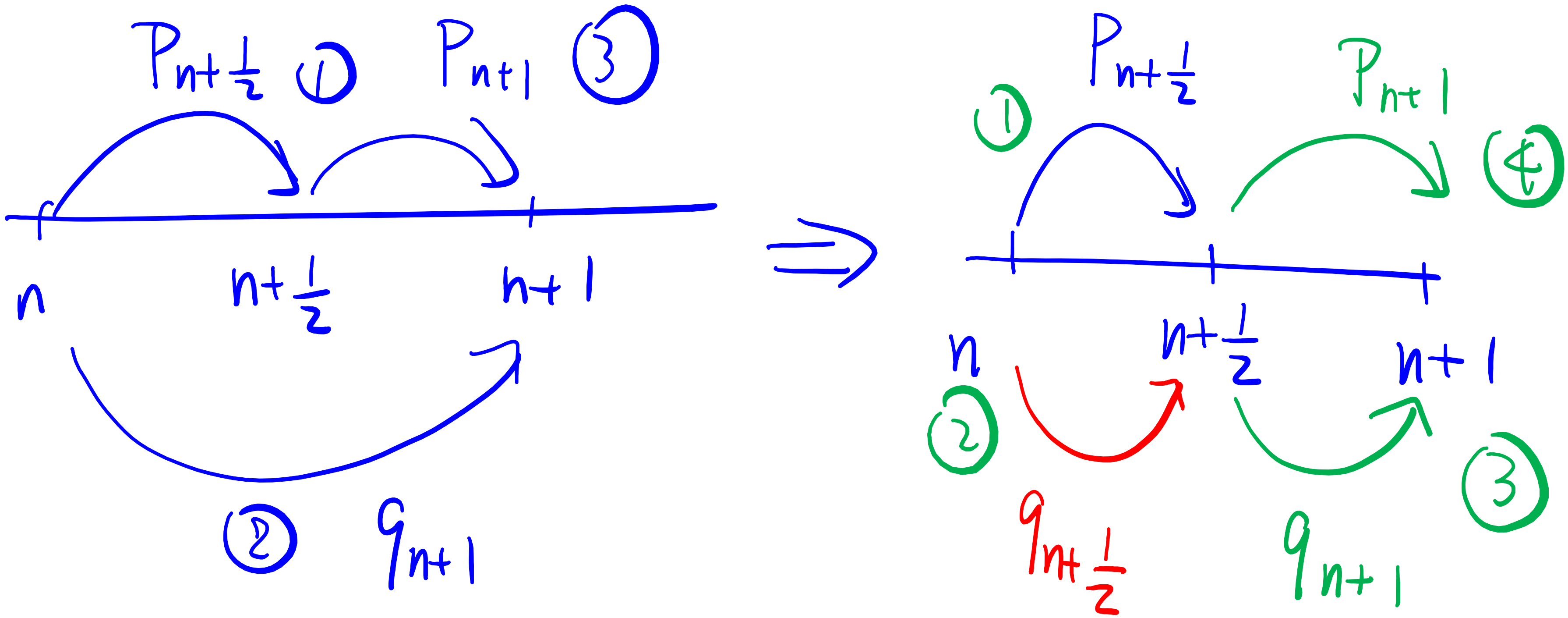
Symplectic Euler (2)

$$\begin{cases} p_{n+1} = p_n - h D_q V(q_{n+1}) \\ q_{n+1} = q_n + h D_p T(p_n) \quad \leftarrow \text{first} \end{cases}$$

Strömer - Verlet.

$$\begin{cases} p_{n+\frac{1}{2}} = p_n - \frac{h}{2} D_q V(q_n) \\ q_{n+1} = q_n + h\left(D_p T(p_{n+\frac{1}{2}})\right) \end{cases}$$

$$p_{n+1} = p_{n+\frac{1}{2}} - \frac{h}{2} \underbrace{D_q V(q_{n+1})}$$



$$\Phi_h^{SV} = \Phi_{\frac{h}{2}}^{SE(2)} \circ \Phi_{\frac{h}{2}}^{SE(1)} \Rightarrow \text{symplectic}.$$

Backward Error analysis.

modified eq.

$$\dot{u} = f(u)$$

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

$$\dot{\tilde{u}} = \tilde{f}_h(\tilde{u}) = f(\tilde{u}) + h f_2(\tilde{u}) + \cdots$$

Ex. Forward Euler.

$$\underbrace{\tilde{u}(t_{n+1})}_{\equiv\, u_{n+1}} = \underbrace{\tilde{u}(t_n)}_{=\, u_n} + h\,\tilde{f}_h(\tilde{u}(t_n))$$

$$+ \frac{h^2}{2}\,\tilde{f}_h'(\tilde{u}(t_n)) \cdot \tilde{f}_h(\tilde{u}(t_n)) + O(h^3)$$

$$
\begin{aligned}
u_{n+1} &= u_n + h\left(f(u_n) + h f_2(u_n) + O(h^2)\right) \\
&\quad + \frac{h^2}{2}\left(f'(u_n) + O(h)\right)\left(f(u_n) + O(h)\right) \\
&\quad + O(h^3) \\
&= u_n + h f(u_n) + h^2 \underbrace{\left(f_2(u_n) + \frac{1}{2} f'(u_n) f(u_n)\right)}_{\substack{\shortparallel \\ 0}} \\
&\quad + O(h^3) \\
&= u_n + h f(u_n)
\end{aligned}
$$

$$f_2(u) = -\frac{1}{2} f'(u) f(u)$$

Similarly obtain $f_3, f_4 \cdots$

Ex. Trapezoidal rule.

$$u_{n+1} = u_n + \frac{h}{2}\left(f(u_n) + f(u_{n+1})\right)$$

$$u_{n+1} = u_n + h\left(f + h f_2 + h^2 f_3 + O(h^3)\right)$$

$$+ \frac{h^2}{2}\left(f' + h f_2' + O(h^2)\right)\left(f + h f_2 + O(h^2)\right)$$

$$+ \frac{h^3}{6}\left(f'' f^2 + f'^2 f + O(h)\right) + O(h^4)$$

Scheme

$$u_{n+1} = u_n + \frac{h}{2}\left(f(u_n) + f(u_{n+1})\right)$$

$$= u_n + \frac{h}{2} f(u_n) + \frac{h}{2} f\left(u_n + \frac{h}{2}\left(f(u_n) + f(u_{n+1})\right)\right)$$

$$= u_n + \frac{h}{2} f + \frac{h}{2}\Big[f + f' \cdot \frac{h}{2}\big(f + f(u_{n+1})\big)$$

$$+ \frac{h^2}{2} f'' f^2 + O(h^3) \Big]$$

$$= u_n + hf + \frac{h^2}{2} f' f + O(h^3)$$

$$\boxed{f_2 = 0}$$

$$f_3 = \frac{1}{12}\left(f'^2 f + f'' f^2 \right)$$

$$\dot{\tilde{u}} = f(\tilde{u}) + h^2 f_3(\tilde{u}) + O(h^3)$$

Thm. p order.

$\Rightarrow f_2 = \cdots = f_p = 0$

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