Lecture 1

$$E_{tot} = \sum_i \frac{m_i v_i^2}{2} + U(r_1 \ldots r_n)$$

Momenta

$$p_i = m_i v_i \,, \quad q^i := r_i$$

$$\boxed{H = \sum_i^N \frac{p_i^2}{2m_i} + U(q^1, \ldots, q^N)}$$

$$\begin{pmatrix} r^1_x \\ r^1_y \\ r^1_z \\ r^2_x \\ r^2_y \\ r^2_z \\ \vdots \\ r^n_z \end{pmatrix} = \begin{pmatrix} q^1 \\ \vdots \\ \vdots \\ q^N \end{pmatrix}$$

$N = 3n$

H – Hamiltonian

$$\begin{cases} \dot{q}^i = \cancel{\frac{p_i}{m_i}} = \frac{\partial H}{\partial p_i} \\ \dot{p}_i = \cancel{-\frac{\partial U}{\partial r_i}} = -\frac{\partial H}{\partial q^i} \end{cases}$$

$$\dot{H}(q,p) = \sum_{i=1}^N \frac{\partial H}{\partial q^i} \dot{q}^i + \sum_{i=1}^N \frac{\partial H}{\partial p_i} \dot{p}_i =$$

$$= \sum_{i=1}^N \left(\frac{\partial H}{\partial q^i} \frac{\partial H}{\partial p_i} + \frac{\partial H}{\partial p_i}\left(-\frac{\partial H}{\partial q^i}\right) \right)$$

$$= 0.$$

That was a simple example of Poisson geometry

$$M = T^*Q \,, \quad C^\infty(M)$$

$p_i \quad q^i$

$$\{\cdot, \cdot\} : C^\infty(M) \times C^\infty(M) \to C^\infty(M)$$

$$\{f, g\} = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right)$$

$$= -\{g, f\}$$

$$\dot{q} = \pm\{q, H\}$$

$$\dot{p} = \pm\{p, H\}$$

$$\dot{f}(q,p) = \pm\{f, H\}$$

$$\dot{H}(q,p) = \{H, H\} = 0$$

Exercise 1

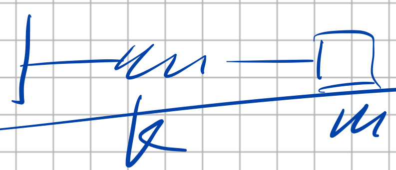
This is also an example of a symplectic space

↳ tomorrow

Exercise 2

1) $H = \frac{q^2}{2} + \frac{p^2}{2}$

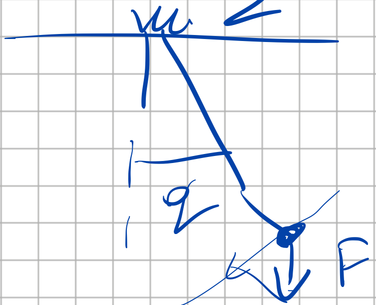
Q: Equations and solve them



$m = k = 1$

2) $H = \frac{p^2}{2} + \cos q^{\cancel{2}}$

Q: Equations and solve them



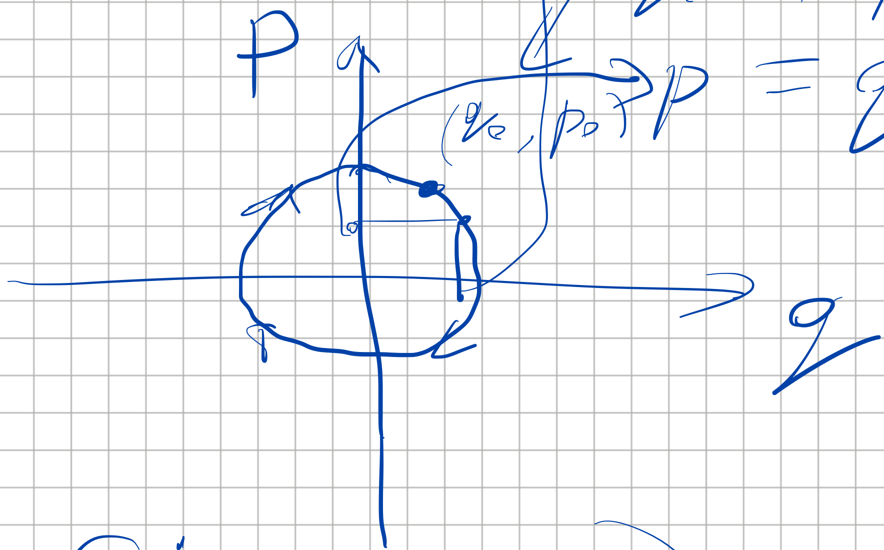
typo, sorry (but does not change the moral)

1) $\begin{cases} \dot{q} = p \\ \dot{p} = -q \end{cases}$ / $\ddot{q} + q = 0$

$\Rightarrow q = A\cos t + B\sin t$

$q(0),\ p(0)$

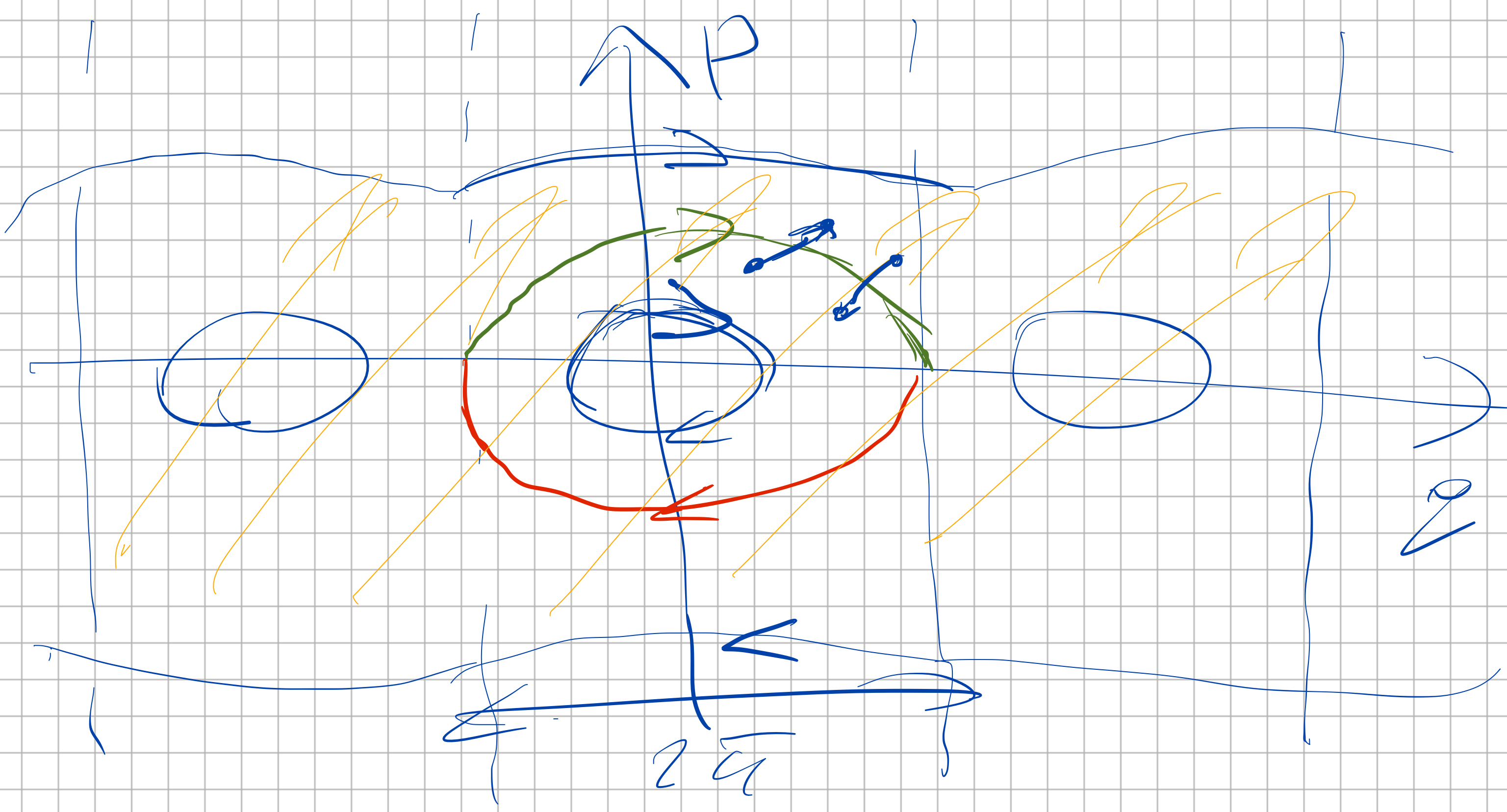
$\Rightarrow p = \dot{q}$



$H = \text{const}$

2) $\begin{cases} \dot{q} = p \\ \dot{p} = \sin q \end{cases}$

Elliptic functions



Lecture 2

$q, v \rightsquigarrow TQ \simeq \mathbb{R}^{2N} = \mathbb{R}^N \times V^N$ (q)

$q, p \rightsquigarrow T^*Q \simeq \mathbb{R}^{2N} = \mathbb{R}^N \times (V^N)^*$

Hamiltonian

$H \longrightarrow \boxed{\{\ \}} \longrightarrow$ system of ODE $\Updownarrow$ a vector field on (T^*Q)

$$X_H = \Big(\underbrace{\frac{\partial H}{\partial p_i}}_{N}, \underbrace{-\frac{\partial H}{\partial q^i}}_{N} \Big)$$

solve the system of ODE $\Longleftrightarrow$ integrate X_H find a curve in T^*Q s.t. X_H is tangent to it.

$$dH = \begin{pmatrix} \frac{\partial H}{\partial q^i} \\ \frac{\partial H}{\partial p_i} \end{pmatrix} \qquad dH = \sum_{i=1}^{N} \left(\frac{\partial H}{\partial q^i} dq^i + \frac{\partial H}{\partial p_i} dp_i \right)$$

They are related by $J = \left(\begin{array}{c|c} 0 & I_N \\ \hline -I_N & 0 \end{array}\right)$

$$X_H = J\, dH$$

$\omega := J^{-1}$

$$dH = \omega(X_H)$$
$$dH = \iota_{X_H} \omega$$

$$\omega = \pm \sum_{i=1}^{N} dq^i \wedge dp_i$$ Exc 1

1) ω is non-degenerate
2) $d\omega = 0$

} symplectic form

- Non deg $\Rightarrow$ $H \to \boxed{\omega} \to X_H$
- Closed $\Rightarrow$ ω is invariant by the flow of X_H

$$\mathcal{L}_{X_H} \omega \underset{\text{Cartan's magic f-la}}{=\!=} (\iota_{X_H} d + d\iota_{X_H})\omega =$$

$$= \underbrace{\iota_X (d\omega)}_{=0} + d(\underbrace{\iota_{X_H}\omega}_{dH}) = 0$$

ω $M \xrightarrow{f} M$
" $f^*(\omega) = \omega$ "

Exercise 2(*)

Given ω, and a diff. eq. ω and a vector field v

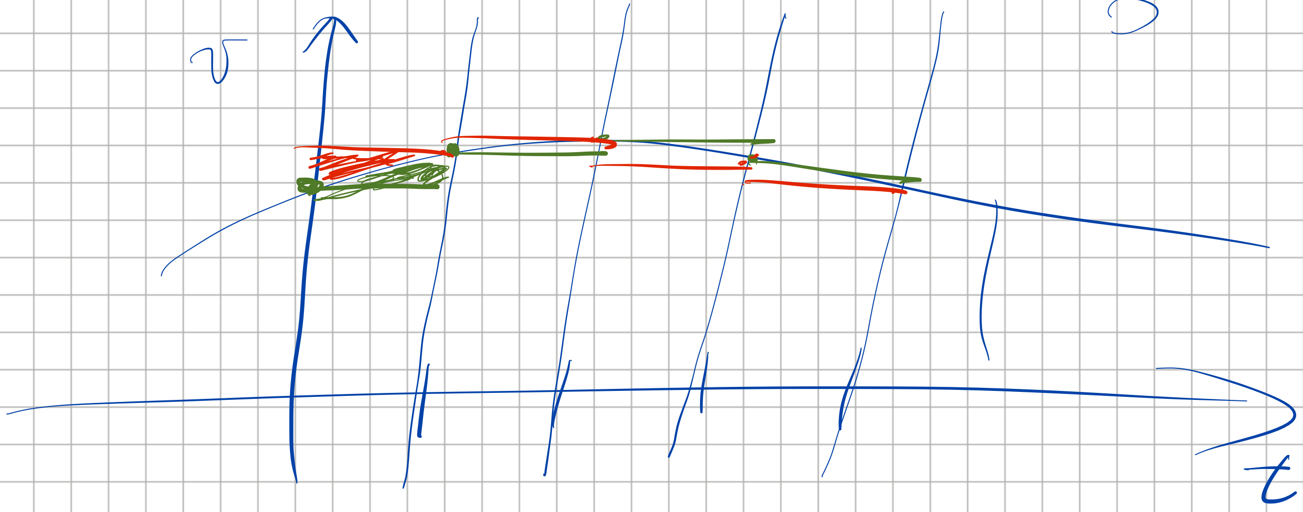
Let us say that v preserves ω

Can we say something about conservation of energy?

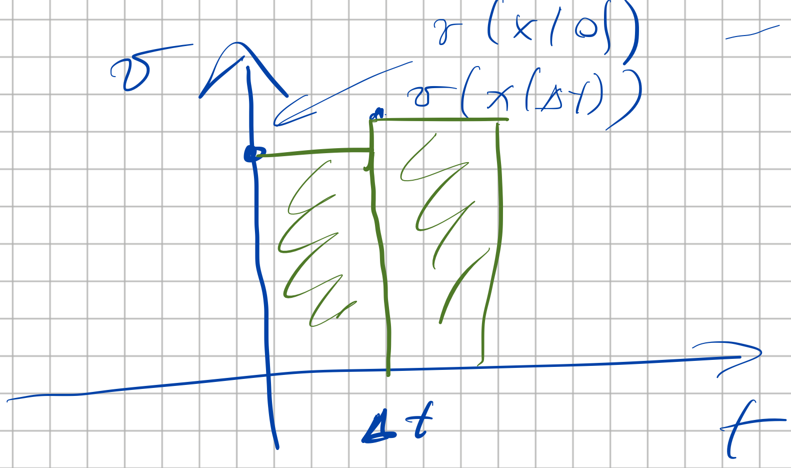
Numerics in 15 minutes

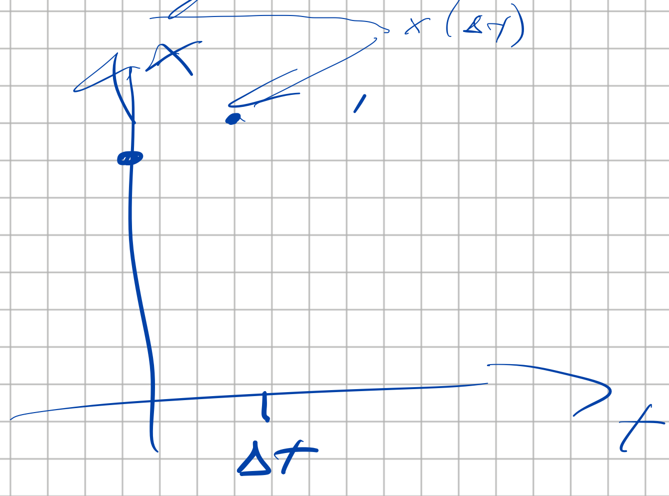
In 1D $\qquad \dot{x} = v(x)$

$$x(T) = x(0) + \int_0^T v(x(t))\,dt$$



$$\int \approx \sum \text{ areas of rectangles}$$





$$x(t+\Delta t) = x(t) + \Delta t \cdot v(x(t))$$

$$= x(t) + \Delta t \cdot v(x(t+\Delta t))$$

Euler Method

$$\boxed{F(x(t+\Delta t)) = 0}$$

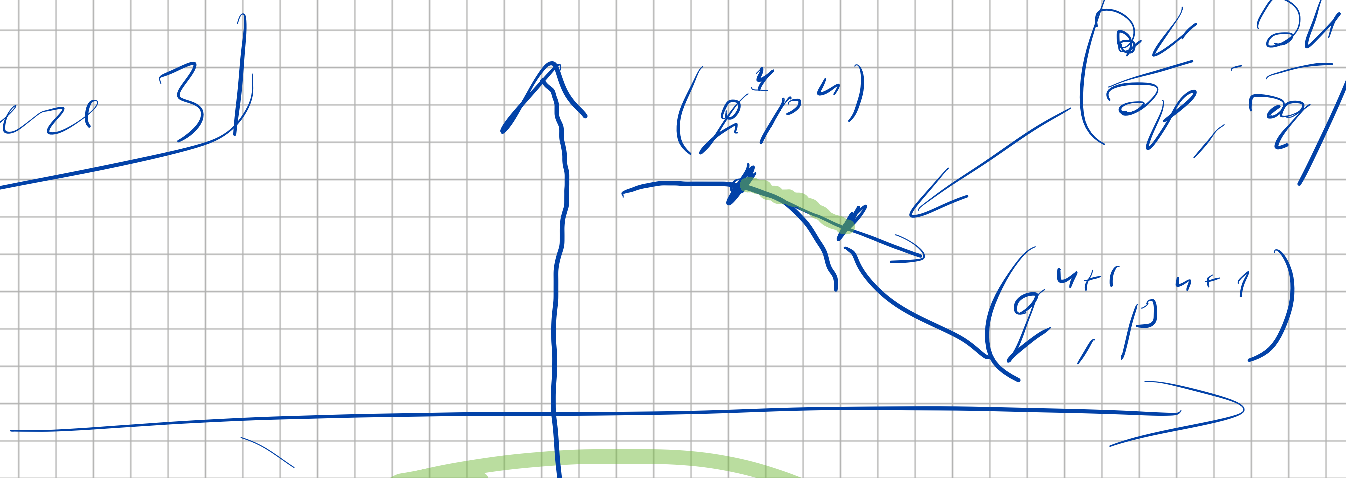
Implicit Euler method

$$x = \begin{pmatrix} q_1 \\ \vdots \\ q_N \\ p_1 \\ \vdots \\ p_N \end{pmatrix} \qquad v = \begin{pmatrix} X_H \end{pmatrix}$$

Exercise 3 (task)

Do this for the examples 1 & 2 from the previous lecture

lecture 3



$$\begin{cases} q^{n+1} = q^n + \Delta t \frac{\partial H}{\partial p}(q^n, p^n) \\ p^{n+1} = p^n + \Delta t \left(-\frac{\partial H}{\partial q}(q^n, p^n)\right) \end{cases}$$

(q^{n+1}, p^{n+1})

(q^{n+1}, p^{n+1})

(q^n, p^{n+1})

(q^n, p^{n+1})

semi-explicit $\rightsquigarrow$ symplectic

- from symplectic forms to energy conservation

$\omega(\cdot,\cdot)$ non degenerate

closed $d\omega = 0$

v – vector field $\quad \mathcal{L}_v \omega = 0 \;(*)$

Q: H – energy, is it conserved by the flow of v?

apriori no

Q: Given $(*)$ can I find an energy that is conserved

$$\iota_v(d\omega) + d(\iota_v\omega) = 0$$

$= 0$

$$\alpha := \iota_v \omega \equiv \omega(v,\cdot)$$

$$d\alpha = 0 \Leftarrow \alpha \overset{?}{=} dH$$

$$d\alpha = 0 \not\Rightarrow \alpha = dH$$

If there is no cohomology at this degree (= there is no difference between closed and exact forms) then $\exists H$.

Suppose $\boxed{\iota_v \omega = dH}$ $\quad v = X_H$

$$\mathcal{L}_v H = \iota_v dH = \iota_v \iota_v \omega = \omega(v,v) = 0$$

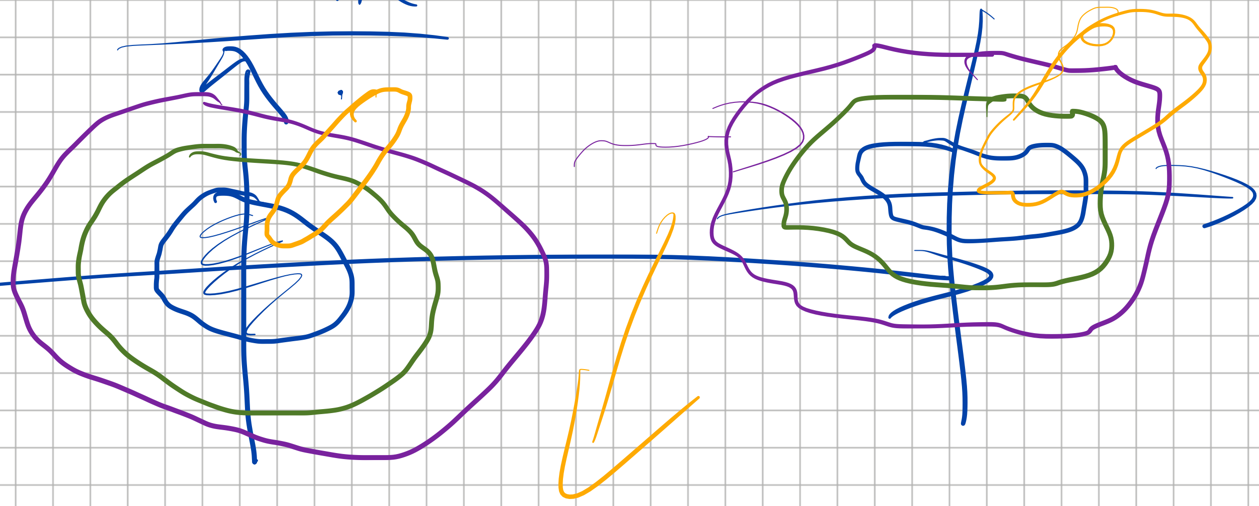
Take home message:

1). v preserving $\omega \Longrightarrow v = X_H$ (if some cond's)

2) if $v = X_H \Longrightarrow v$ preserves the level sets of H

Interpretation in 2D

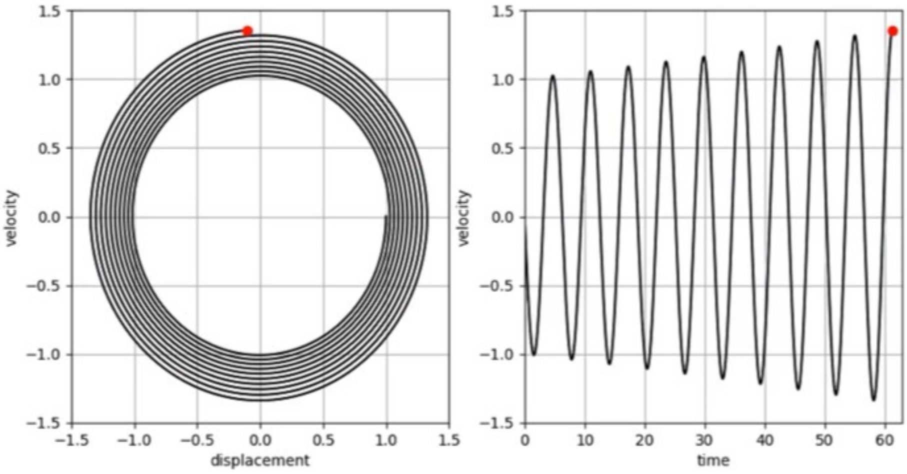
ω — is the (oriented) area in $\mathbb{R}^2$



preserve level sets

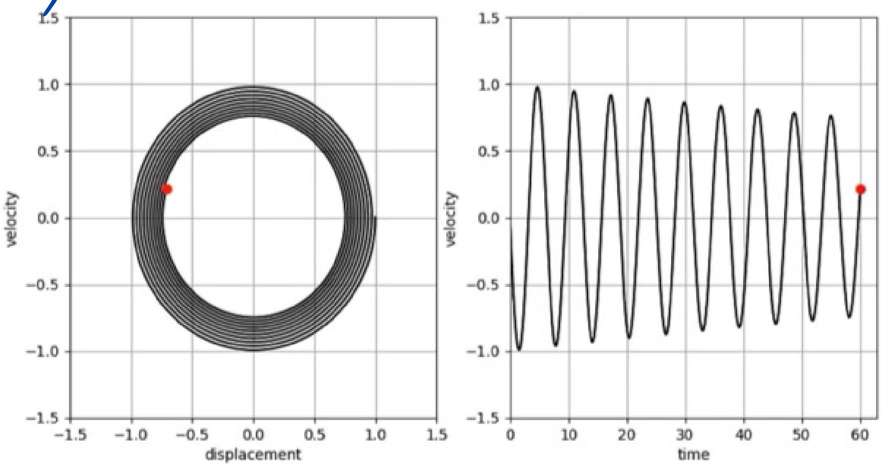
Explicit Euler for $H = \frac{q^2}{2} + \frac{p^2}{2}$

$$\begin{cases} q^{n+1} = q^n + \Delta t \frac{\partial H}{\partial p}(q^n, p^n) \\ p^{n+1} = p^n + \Delta t\left(-\frac{\partial H}{\partial q}(q^n, p^n)\right) \end{cases}$$



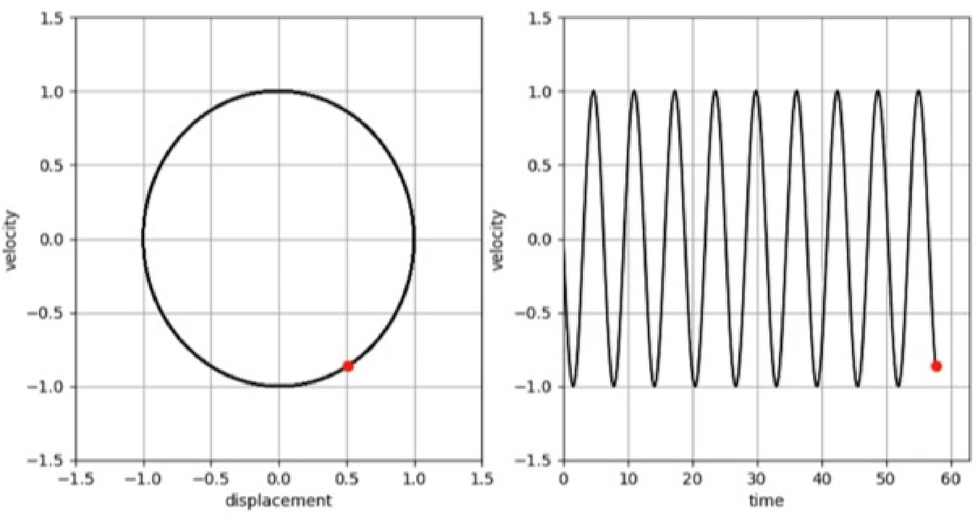
Implicit Euler

$$\begin{cases} q^{n+1} = q^n + \Delta t \frac{\partial H}{\partial p}(q^{n+1}, p^{n+1}) \\ p^{n+1} = p^n + \Delta t\left(-\frac{\partial H}{\partial q}(q^{n+1}, p^{n+1})\right) \end{cases}$$



Symplectic Euler

$$\begin{cases} q^{n+1} = q^n + \Delta t \frac{\partial H}{\partial p}(q^n, p^{n+1}) \\ p^{n+1} = p^n + \Delta t\left(-\frac{\partial H}{\partial q}(q^n, p^{n+1})\right) \end{cases}$$



Further reading

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3. *D. Razafindralandy, A. Hamdouni, M. Chhay*, A review of some geometric integrators // Advanced Modeling and Simulation in Engineering Sciences, SpringerOpen, 2018, 5 (1), pp.16.

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Thank you for attention!