Classical Statistical Mechanics &

Computer Simulations

Lagrangian Mechanics

Newton's eq. of motion:

$$m_i \ddot{\vec{r}}_i = \vec{F}_i = -\frac{\partial U}{\partial \vec{r}_i} \qquad U = U(\{\vec{r}_i\})$$

$$E_{kin} = \sum_i \frac{1}{2} m_i \dot{\vec{r}}_i^{\,2}$$

$$L = E_{kin} - U = L(\{\vec{r}_i\}, \{\dot{\vec{r}}_i\})$$

Lagrange function, "Lagrangian"

$$\frac{\partial L}{\partial \vec{r}_i} = -\frac{\partial U}{\partial \vec{r}_i} = \vec{F}_i \qquad \frac{\partial L}{\partial \dot{\vec{r}}_i} = \frac{\partial}{\partial \dot{\vec{r}}_i} E_{kin} = \underbrace{m_i \dot{\vec{r}}_i}_{\text{momentum}}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec{r}}_i}\right) = m_i \ddot{\vec{r}}_i \Rightarrow \boxed{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec{r}}_i}\right) = \frac{\partial L}{\partial \vec{r}_i}}$$

$$L = E_{kin} - U = L(\{\vec{r}_i\}, \{\dot{\vec{r}}_i\})$$

Lagrange function, "Lagrangian"

$$\frac{\partial L}{\partial \vec{r}_i} = -\frac{\partial U}{\partial \vec{r}_i} = \vec{F}_i \qquad \frac{\partial L}{\partial \dot{\vec{r}}_i} = \frac{\partial}{\partial \dot{\vec{r}}_i} E_{kin} = m_i \dot{\vec{r}}_i$$

momentum

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec{r}}_i}\right) = m_i \ddot{\vec{r}}_i \Rightarrow \boxed{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\vec{r}}_i}\right) = \frac{\partial L}{\partial \vec{r}_i}}$$

SO WHAT ??

Euler-Lagrange equation

Calculus of Variations

"Function of a function": FUNCTIONAL

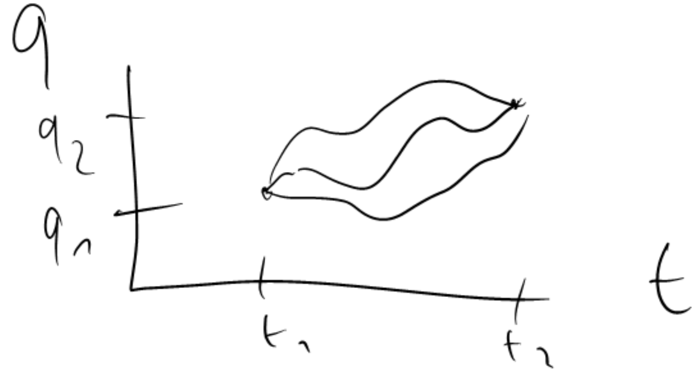
$S[q(t)]$: $q(t)$ is unknown, $S[q(t)]$ is KNOWN.

IDEA: Pick $q(t)$ such that $S[q(t)] \stackrel{!}{=} \text{Min}$.

$$S = \int_{t_1}^{t_2} dt \, L(q, \dot{q})$$

boundary cond.

$$q(t) = \begin{cases} q_1 & t = t_1 \\ q_2 & t = t_2 \end{cases}$$



ACTION.

Principle of least action

Hamilton's principle

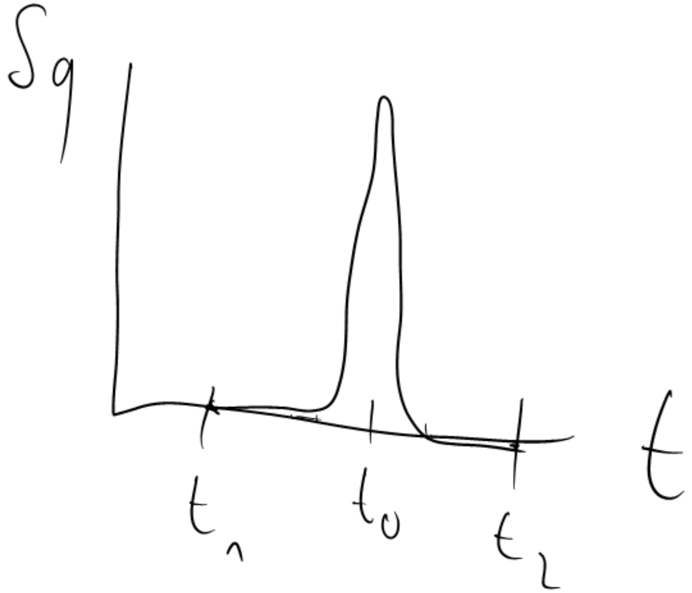
$$q(t) = \underbrace{q_0(t)}_{\text{Solution of the problem}} + \underbrace{\delta q(t)}_{\text{deviation}} \qquad \delta S = 0$$

$$\delta S = \delta \int_{t_1}^{t_2} dt\, L(q, q) = \int_{t_1}^{t_2} dt \left[\frac{\partial L}{\partial \dot q} \delta \dot q + \frac{\partial L}{\partial q} \delta q \right] :$$

$$= \int_{t_1}^{t_2} dt \left[\frac{\partial L}{\partial \dot q} \frac{d}{dt} \delta q + \frac{\partial L}{\partial q} \delta q \right] \underset{\text{partial integr.}}{=}$$

$$= \int_{t_1}^{t_2} dt \left[-\frac{d}{dt}\left(\frac{\partial L}{\partial \dot q} \right) \delta q + \frac{\partial L}{\partial q} \delta q \right] + \underbrace{\frac{\partial L}{\partial \dot q} \delta q \Big|_{t_1}^{t_2}}_{=0}$$

$$= \int_{t_1}^{t_2} dt \left[\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right)\right] \delta q \overset{!}{=} 0$$ for ANY δq



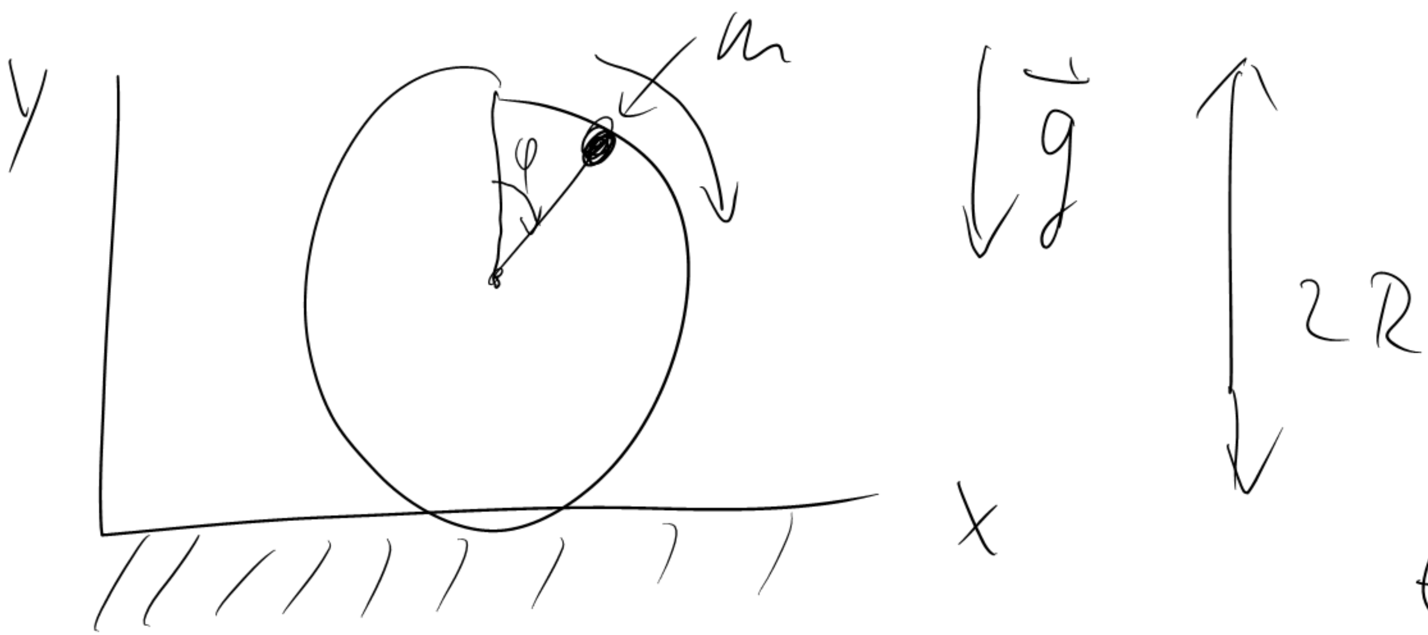
$$\Rightarrow \boxed{\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0}$$

Euler-Lagrange eq.

Several functions q_i: $$\boxed{\frac{\partial L}{\partial q_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = 0}$$

Useful: easy coordinate transformations!

Example: Wheel with a mass point



$$g = 9.81\,\frac{m}{s^2}$$

$t > 0$:

$$t = 0: \quad \begin{pmatrix} x \\ y \end{pmatrix} = \vec{r} = \begin{pmatrix} 0 \\ 2R \end{pmatrix}$$

$$\vec{r} = \begin{pmatrix} R\varphi \\ R \end{pmatrix} + \begin{pmatrix} R\sin\varphi \\ R\cos\varphi \end{pmatrix} = R\begin{pmatrix} \varphi + \sin\varphi \\ 1 + \cos\varphi \end{pmatrix}$$

$$\dot{\vec{r}} = R\begin{pmatrix} \dot\varphi + \dot\varphi\cos\varphi \\ -\sin\varphi\,\dot\varphi \end{pmatrix} = R\dot\varphi\begin{pmatrix} 1 + \cos\varphi \\ -\sin\varphi \end{pmatrix}$$

$$\dot{\vec{r}}^2 = R^2\dot\varphi^2\left[(1+\cos\varphi)^2 + \sin^2\varphi\right] =$$

$$= \left[1 + 2\cos\varphi + \cos^2\varphi + \sin^2\varphi\right] R^2\dot\varphi^2 =$$

$$= 2R^2\dot\varphi^2\,(1+\cos\varphi)$$

$$\left.\begin{aligned} E_{kin} &= mR^2\dot{\varphi}^2(1+\cos\varphi) \\ U &= mgR\cos\varphi \end{aligned}\right\} L = mR^2\dot{\varphi}^2(1+\cos\varphi) - mgR\cos\varphi$$

$$\frac{\partial L}{\partial \dot{\varphi}} = 2mR^2\dot{\varphi}(1+\cos\varphi) \qquad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\varphi}}\right) = 2mR^2\ddot{\varphi}(1+\cos\varphi) + 2mR^2\dot{\varphi}(-\sin\varphi)\dot{\varphi}$$

$$\frac{\partial L}{\partial \varphi} = mgR\sin\varphi - mR^2\dot{\varphi}^2\sin\varphi$$

$$\Rightarrow \quad 2mR^2\ddot{\varphi}(1+\cos\varphi) - 2mR^2\dot{\varphi}^2\sin\varphi = mgR\sin\varphi - mR^2\dot{\varphi}^2\sin\varphi$$

$$2\cancel{m} R^2 \ddot{\varphi} (1+\cos\varphi) = \cancel{m} R^2 \sin\varphi \left(\dot{\varphi}^2 + \frac{g}{R}\right)$$

$$\boxed{\ddot{\varphi} = \left(\frac{g}{R} + \dot{\varphi}^2\right) \frac{\sin\varphi}{2(1+\cos\varphi)}}$$

energy theorem: $E_{tot} = E_{kin} + U =$

$$= m R^2 \dot{\varphi}^2 (1+\cos\varphi) + mgR\cos\varphi$$

$$\dot{\varphi}^2 = \frac{E_{tot} - mgR\cos\varphi}{mR^2(1+\cos\varphi)} = \left(\frac{d\varphi}{dt}\right)^2$$

$$\Rightarrow \quad \frac{d\varphi}{dt} = \sqrt{\frac{E_{tot} - mgR\cos\varphi}{mR^2(1+\cos\varphi)}}$$

$$\underbrace{\int dt}_{t \,+\, \text{const.}} = \underbrace{\int d\varphi \sqrt{\frac{mR^2(1+\cos\varphi)}{E_{tot} - mgR\cos\varphi}}}_{\text{function}(\varphi)} \Rightarrow t(\varphi)$$

$$\xRightarrow[\text{invert}]{} \varphi(t) \text{ solution}$$

Energy theorem in Lagrangian mechanics

Energy is conserved $\iff$ U does not depend on time

$\Rightarrow$ L does not depend explicitly on time, (explicitly)

$$\frac{\partial L}{\partial t} = 0 \, .$$

ONE degree of freedom:

$$L = L(q, \dot{q}, \cancel{t})$$

eq. motion

$$\frac{dL}{dt} = \frac{\partial L}{\partial q}\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right)\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q} =$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot q}\dot q\right) = \frac{dL}{dt} \Rightarrow \frac{d}{dt}\left(\frac{\partial L}{\partial \dot q}\dot q - L\right) = 0$$

$$\Rightarrow \frac{\partial L}{\partial \dot q}\dot q - L = E_{tot} = \text{const.}$$

many degrees of freedom: $E_{tot} = \sum_i \left(\frac{\partial L}{\partial \dot q_i}\dot q_i\right) - L$

$$L = \frac{1}{2}\sum_i m_i \dot{\vec r}_i^{\,2} - U$$

$$\frac{\partial L}{\partial \dot{\vec r}_i} = m_i \dot{\vec r}_i \quad \sum_i \dot{\vec r}_i \cdot \frac{\partial L}{\partial \dot{\vec r}_i} = \sum_i m_i \dot{\vec r}_i^{\,2} = 2E_{kin}$$

$$\sum_i \left(\frac{\partial L}{\partial \dot{\vec{r}}_i} \cdot \dot{\vec{r}}_i \right) - L = 2E_{kin} - (E_{kin} - U) =$$

$$= E_{kin} + U = E_{tot}$$

Constraints & Generalized Coordinates

Constraint forces: We do NOT know the force,

BUT we know in what it results!

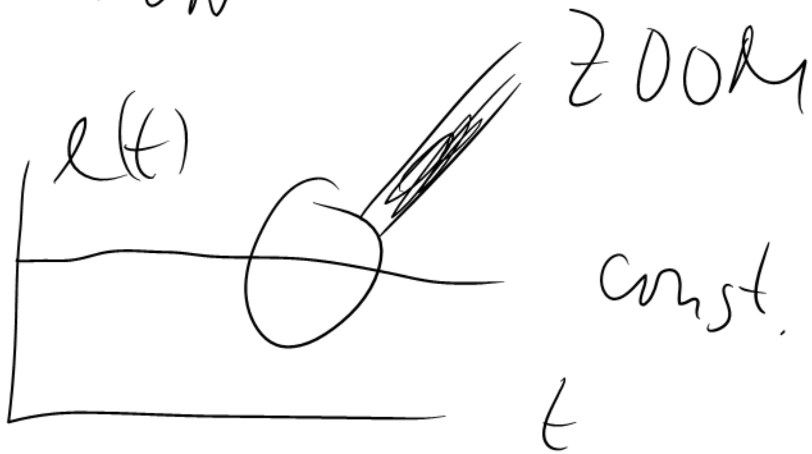
Consider so-called HOLONOMIC constraints:

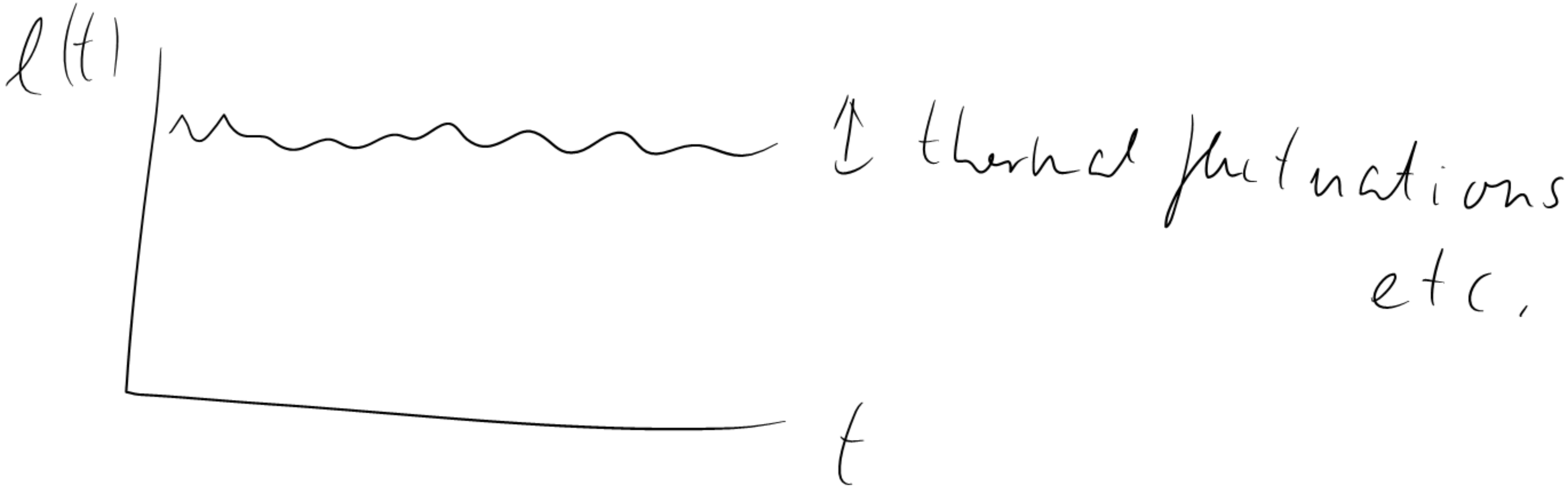
$$G_i(\{\vec{r}_j\}) = 0 \to \text{trajectory is confined to a manifold}$$

in reality: There ARE NO constraints!

Constraint $\equiv$ IDEALIZATION

example: Rigid rod



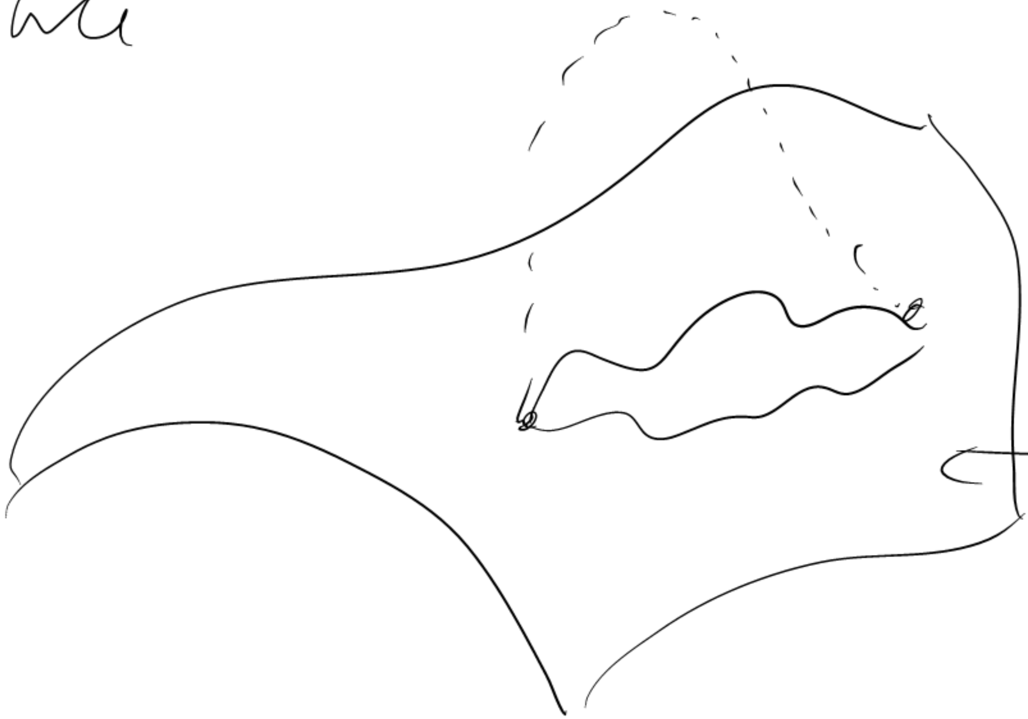


constraint force $\equiv$ idealization for the internal elastic forces

$S \overset{!}{=}$ Min.

constraints confine the trajectory

q space



constraint surface

 : trajectories <u>within</u> the surface

 trajectory outside

DISCARD

Find minimums
in the constr. surface!

Method 1: Generalized coordinates:

Find a set of parameters q_i such that

↳ coord. within the surface

$$G_k\left(\left\{\vec{r}_i(q_j)\right\}\right) = 0$$

$$\Rightarrow L = L\left(\{q_i\}\{\dot{q}_i\}\right)$$