PHY 321 APRIL 19

why is Lagrangian + Variational calculus so powerful?

$\mathcal{L} = K - V$

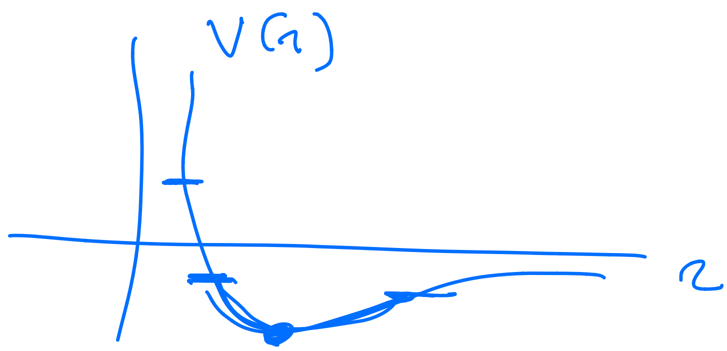
Euler-Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} = 0$$

$\Rightarrow$ equations of motion and Newton's

HW 6

Lennard-Jones potential



$$V(r) = V_0\left(\left(\frac{a}{r}\right)^{12} - \left(\frac{b}{r}\right)^{6}\right)$$

$r = |\vec{r}_1 - \vec{r}_2|$

polar coordinates

$r \in [0, \infty) \quad \phi \in [0, 2\pi]$

$$K = \underline{\tfrac{1}{2}\mu}(\dot{r}^2 + r^2\dot{\phi}^2) \qquad \dot{r} = \frac{dr}{dt}$$

$$\frac{dV}{dr} = -6V_0\left(\underbrace{2\frac{a^{12}}{r^{13}} - \frac{b^6}{r^7}}\right)$$

$$\frac{\partial \mathcal{L}}{\partial r} = r\mu\dot{\phi}^2 + 6V_0[\quad]$$

$$\frac{\partial \mathcal{L}}{\partial \dot{r}} = \underline{\mu}\dot{r} \qquad \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{r}} = \mu\ddot{r}$$

$$\ddot{r} = \underbrace{\frac{\mu r\dot{\phi}^2}{\mu}} + \frac{6V_0}{\mu}\left(\frac{2a^{12}}{r^{13}} - \frac{b^6}{r^7}\right)$$

$$\dot{\phi} = \mu r^2 L$$

For many particles a cartesian system is more straightforward to implement

$$\vec{r}_i = (x_i, y_i, z_i)$$

$$K = \sum_{i=1}^{N} \frac{1}{2}\underline{m_i \dot{\vec{r}}_i^{\,2}}$$

N

. . . . .

$$V = \sum_{i=1} \sum_{j \neq i} V(\vec{r}_i - \vec{r}_j)$$

<u>HW 6</u>

$$\vec{\nabla}_i V = -\sum_{j \neq i} 6V_0 \left[2\left(\frac{a}{r}\right)^{12} - \left(\frac{b}{r}\right)^{6} \right] \times \frac{[\vec{r}_i - \vec{r}_j]}{r^2}$$

$$\frac{\partial \mathcal{L}}{\partial \vec{r}_i} = - \vec{\nabla}_i V$$

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{r}}_i} = m_i \ddot{\vec{r}}_i$$

$$\ddot{\vec{r}}_i = - \frac{6V_0}{m_i} \sum_{j \neq i} \left[\qquad \right] \times \frac{[\vec{r}_i - \vec{r}_j]}{r^2}$$

$$\frac{\partial \mathcal{L}}{\partial \dot{\vec{r}}_i} = m_i \dot{\vec{r}}_i$$

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\vec{r}}_i} = m_i \ddot{\vec{r}}_i$$

Example 2

Harmonic oscillations

friction : $\vec{f}_R = -b \frac{dx}{dt}$

$$2\lambda = \frac{b}{m}$$

$$\ddot{x} + 2\lambda \dot{x} + w_0^2 x = 0$$

is this general law ?

No.

$\vec{F} = -\vec{\nabla} V(\vec{r})$ (line integrals)

Friction is not a conservative force.

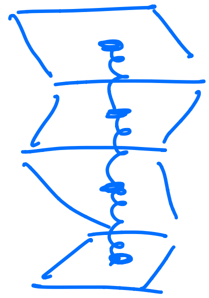
To Euler-Lagrange we simply add $\vec{f}_R$:

$$\frac{\partial L}{\partial \vec{r}} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\vec{r}}} + \vec{f}_R = 0$$

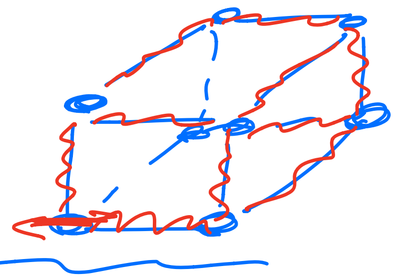
Example 3

Coupled Harmonic oscillator

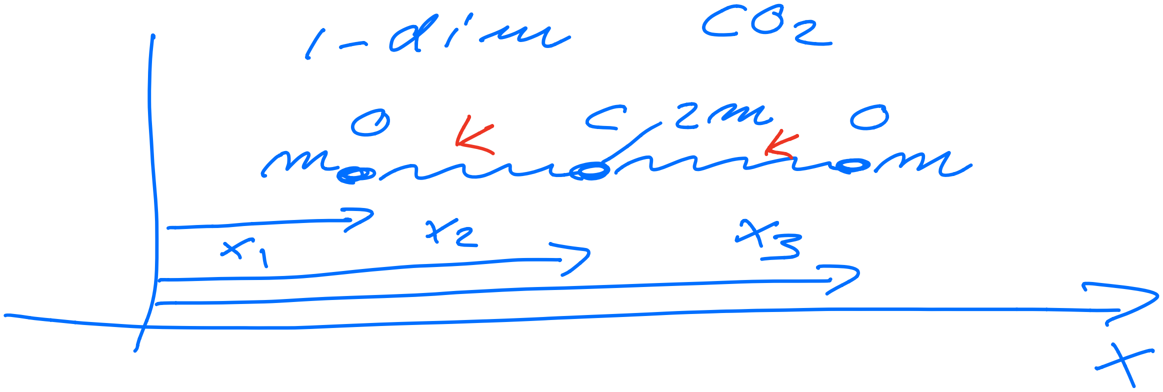
– Earthquake models



\- Materials Science



\- Molecule model in 1-dim CO_2



$$\mathcal{L} = \frac{1}{2} m \dot{x}_1^2 + m \dot{x}_2^2 + \frac{1}{2} m \dot{x}_3^2 - \frac{k}{2}(x_2 - x_1 - \ell)^2 - \frac{k}{2}(x_3 - x_2 - \ell)^2$$

ℓ = relaxed lengths of both springs.

$$\frac{\partial L}{\partial x_i} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}_i} = 0$$

$$m\ddot{x}_1 = -k(x_1 - x_2 + \ell)$$

$$2m\ddot{x}_2 = -k(x_2 - x_1 - \ell) + k(x_2 - x_3 + \ell)$$

$$m\ddot{x}_3 = -k(x_3 - x_2 + \ell)$$