Last class : $F_x^{net} = m a_x$

<u>Euler Step</u> :

$$v_x(t+\Delta t) = v_x(t) + \frac{F_x^{net}}{m}\Delta t$$

$$x(t+\Delta t) = x(t) + \underbrace{v_x(t)}_{v_x(t+\Delta t)}\Delta t$$

<u>Euler-Cromer Step:</u>

$$F_x^{net} = -kx$$

$$E_{tot} = \frac{1}{2}kx^2 + \frac{1}{2}m v_x^2$$

Solution : $t_0=0 \quad v_0=0$

$$x(t) = x_0 \cos(\omega_0 t)$$

$$y(t) = -x_0\omega_0 \sin(\omega_0 t)$$

where $\omega_0 = \sqrt{\frac{k}{m}}$

Explanation for divergence of E for Euler Step

$$E(t+\Delta t) = \frac{1}{2}k\, x(t+\Delta t)^2 + \frac{1}{2}m\left(v_x(t+\Delta t)\right)^2$$

$$= \frac{1}{2}k\left(x(t) + v_x(t)\Delta t\right)^2 + \frac{1}{2}m\left(v_x(t) - \frac{k}{m}x(t)\Delta t\right)^2$$

$$= \frac{1}{2}k\left[(x(t))^2 + 2x(t)v_x(t)\Delta t + (v_x(t))^2(\Delta t)^2\right] + \frac{1}{2}m\left[(v_x(t))^2 - 2\frac{k}{m}v_x(t)x(t)\Delta t + \left(\frac{k}{m}\right)^2(x(t))^2(\Delta t)^2\right]$$

$$= \underbrace{\frac{1}{2}k(x(t))^2 + \frac{1}{2}m(v_x(t))^2} + \frac{1}{2}k(v_x(t))^2(\Delta t)^2 + \frac{1}{2}\frac{k^2}{m}(x(t))^2(\Delta t)^2$$

$$= \overbrace{E(t)} + \left(\frac{1}{2}k(x(t))^2 + \frac{1}{2}m(v_x(t))^2\right)\frac{k}{m}(\Delta t)^2$$

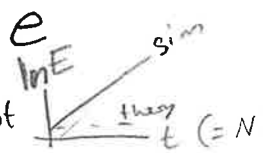
$$= E(t) + E(t)\frac{k}{m}(\Delta t)^2$$

$$E(t+\Delta t) = E(t)\underbrace{\left(1 + \frac{k}{m}(\Delta t)^2\right)}_{>0}$$

(after N timesteps)

$$E(t=N\Delta t) = \underbrace{E(t_0)}_{E_0}\left(1 + \frac{k}{m}(\Delta t)^2\right)^N = E_0\, e^{N\overbrace{\ln\left(1+\frac{k}{m}(\Delta t)^2\right)}^{>0}}$$

→ plot



Euler Cromer check Energy

$$E(t+\Delta t) = \frac{1}{2}k\left(x(t+\Delta t)\right)^2 + \frac{1}{2}m\left(v_x(t+\Delta t)\right)^2$$

$$= \frac{1}{2}k\left[x(t) + v_x(t+\Delta t)\,\Delta t\right]^2 + \frac{1}{2}m\left[v_x(t) - \frac{k}{m}x(t)\Delta t\right]^2$$

$$= \underbrace{\boxed{\frac{1}{2}k(x(t))^2 + \frac{1}{2}m(v_x(t))^2}}_{E(t)} + k\,x(t)\,v_x(t+\Delta t)\,\Delta t + \frac{1}{2}k(v_x(t+\Delta t))^2(\Delta t)^2 - k\,v_x(t)\,x(t)\Delta t + \frac{1}{2}\frac{k^2}{m}(x(t))^2(\Delta t)^2$$

$$= E(t) + k\,x(t)\left[\cancel{v_x(t)} - \frac{k}{m}x(t)\Delta t\right]\Delta t + \frac{1}{2}k\left(v_x(t+\Delta t)\right)^2\Delta t^2 - k\,\cancel{v_x(t)x(t)}\,\Delta t + \frac{1}{2}\frac{k^2}{m}(x(t))^2(\Delta t)^2$$

$$= E(t) - \frac{1}{2}\frac{k^2}{m}(x(t))^2\Delta t^2 + \frac{1}{2}k\left(v_x(t+\Delta t)\right)^2\Delta t^2$$

$$= E(t) - \frac{k}{m}\left[\frac{1}{2}k(x(t))^2 + \frac{1}{2}m\{\overbrace{v_x(t+\Delta t)}^{v_x(t) - \frac{k}{m}x(t)\Delta t}\}^2\right]\Delta t^2$$

$$= E(t) - \frac{k}{m}\left[\frac{1}{2}k(x(t))^2 + \frac{1}{2}m\left\{(v_x(t))^2 - 2v_x(t)\frac{k}{m}x(t)\Delta t + \frac{k^2}{m^2}(x(t))^2\Delta t^2\right\}\right]\Delta t^2$$

$$E(t+\Delta t) = E(t) - \frac{k}{m}\left[E(t) - k\,x(t)\,v_x(t)\,\Delta t + \frac{1}{2}\frac{k^2}{m}(x(t))^2\Delta t^2\right]\Delta t^2$$

$$= E(t)\left\{1 - \frac{k}{m}(\Delta t)^2\right\} + O(\Delta t^3)$$

after N steps

$$E(t+N\Delta t) = E(t_0)\left(1 - \frac{k}{m}(\Delta t)^2\right)^N$$

$$= E(t_0)\,e^{N\ln\left(1 - \frac{k}{m}(\Delta t)^2\right)}$$

$\boxed{\text{Molecular Dynamics Simulation}}$

So far Euler Step:

$$x(t+\Delta t) = x(t) + v_x(t)\,\Delta t$$
$$v_x(t+\Delta t) = v_x(t) + \frac{F_x^{net}}{m}\,\Delta t$$

1dim $\longrightarrow$ d dimensional (2dim. or 3dim.)

$$x \longrightarrow \vec{r}$$
$$v_x \longrightarrow \vec{v}$$
$$a_x = F_x^{net}/m \longrightarrow \vec{F}^{net}/m$$

one particle to many particles

$i = 1, 2, \ldots, N$ particles

$$\vec{r} \longrightarrow \vec{r}_i$$
$$\vec{v} \longrightarrow \vec{v}_i$$
$$\vec{a} \longrightarrow \frac{\vec{F}_i^{net}}{m}$$

special case $\vec{F}_i^{net} = \sum_{j \neq i} \vec{F}_{ij}$