$\boxed{\text{April 1, 2021}}$

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

Euler Step :
$$v_x(t+\Delta t) = v_x(t) + \frac{F_x^{net}}{m} \Delta t$$
$$x(t+\Delta t) = x(t) + \underbrace{v_x(t)}_{v_x(t+\Delta t)} \Delta t$$

Euler-Cromer Step:

$$F_x^{net} = -kx$$
$$E_{tot} = \frac{1}{2} k x^2 + \frac{1}{2} m v_x^2$$

Solution : $t_0 = 0$ $v_0 = 0$
$$x(t) = x_0 \cos(\omega_0 t)$$
$$v(t) = -x_0 \omega_0 \sin(\omega_0 t)$$
where
$$\omega_0 = \sqrt{\frac{k}{m}}$$

Explanation for divergence of E for Euler Step

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

(after N timesteps

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

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

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