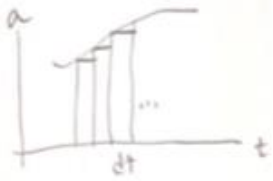
Numerical integration to solve differential eq'ns w/ initial condition

$\frac{d^2x}{dt^2} = -\frac{k}{m}x$, $x(0) = 0$, $v(0) = v_0 \rightarrow a(0) = 0$ — simple harmonic oscillator

Euler (or "first-order") integration



- divide time into steps of length dt
- get solution at $t+dt$ from solution at time t
- assume a is const in each interval dt, then



$v(dt) = v(0) + a(0)\,dt = v_0$

$v(t+dt) = v(t) + a(t)dt$ error dt^2

$x(dt) = x(0) + v(0)dt + \frac{1}{2}a(0)\,dt^2 = v_0\,dt$

$x(t+dt) = x(t) + v(t)\,dt + \frac{1}{2}a(t)\,dt^2$ error dt^3

Better method - Verlet algorithm

consider $x(t+dt) = x(t) + v(t)dt + \frac{1}{2}a(t)\,dt^2$ ①

\+ $x(t-dt) = x(t) - v(t)dt + \frac{1}{2}a(t)\,dt^2$ ② (odd terms cancel)

$x(t+dt) + x(t-dt) = 2x(t) + a(t)\,dt^2$

$$\boxed{x(t+dt) = 2x(t) - x(t-dt) + a(t)\,dt^2}$$ error on positions $\sim dt^4$ per step

velocity: ① - ②

$x(t+dt) - x(t-dt) = 2v(t)\,dt$

$$v(t) = \frac{x(t+dt) - x(t-dt)}{2dt}$$ error on velocity $\sim dt^2$ per step (dt^3/dt)

First time step $t = 0 \Rightarrow dt$, need to know $x(-dt)$

$x(-dt) = x(0) - v(t)\,dt + \frac{1}{2}a(0)\,dt^2$

Reduced units (see Tab. 6.1)

$$\varphi^*(r^*) = 4\left[\left(\frac{1}{r^*}\right)^{12} - \left(\frac{1}{r^*}\right)^{6}\right]$$

$\varphi^* = \varphi/\varepsilon$

$r^* = r/\sigma$

All energies in units of $1/\varepsilon$

$E^* = E/\varepsilon$

$U^* = U/\varepsilon$

$K^* = K/\varepsilon$

other quantities:

$\langle K \rangle = \frac{3}{2} N k_B \langle T \rangle$, so $\boxed{T^* = \frac{k_B T}{\varepsilon}}$

if one type of atom, $m^* = 1$

$\langle K^* \rangle = \frac{3}{2} N \langle T^* \rangle$

time: can find in reduced units using KE

$$\frac{K}{K^*} = \varepsilon = \frac{\frac{1}{2}mv^2}{\frac{1}{2}m^*v^{*2}} = \frac{m\left(\frac{x}{t}\right)^2}{\left(\frac{x^*}{t^*}\right)^2} = m\left(\frac{x}{x^*}\right)^2\left(\frac{t^*}{t}\right)^2$$

$$\varepsilon = m\sigma^2\left(\frac{t^*}{t}\right)^2$$

$$t^* = \frac{t}{\sigma\sqrt{m/\varepsilon}} = \frac{t}{t_0}$$

e.g. calc. t^* for Ar

$\varepsilon_{Ar} = 0.0104$ eV $m_{Ar} = 39.948$ u

$\sigma_{Ar} = 3.4$ Å

convert all to SI units