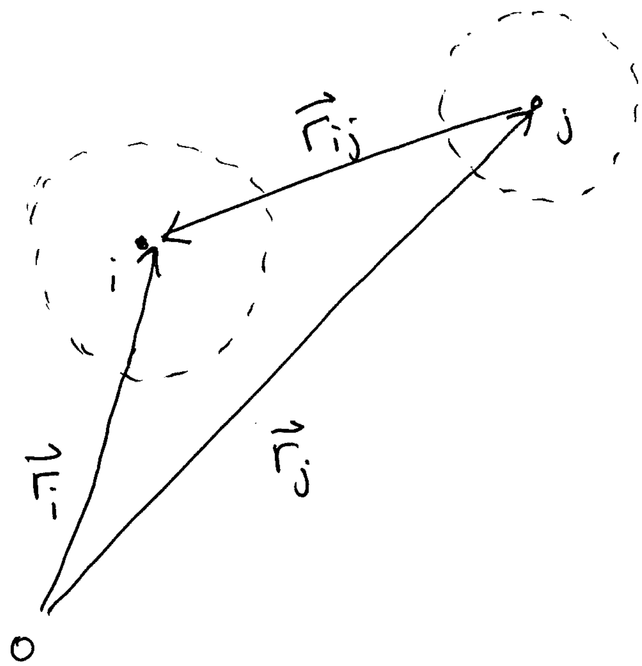
Pair Potentials



$$\vec{r}_i = \vec{r}_j + \vec{r}_{ij}$$

$$\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$$

$$= (x_i - x_j)\,\hat{x} + (y_i - y_j)\,\hat{y}$$

points from j to i

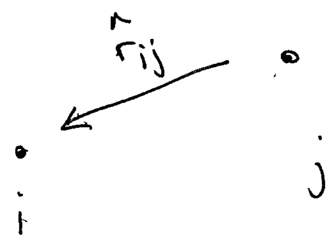
Central Forces

$$\vec{F}_{ij} = \underset{F_{ij}}{(\;)}\,\hat{r}_{ij}$$

$$\hat{r}_{ij} = \frac{\vec{r}_{ij}}{r_{ij}} = \frac{x_{ij}\,\hat{x} + y_{ij}\,\hat{y}}{r_{ij}}$$

force on i due to j

$$\hat{r}_{ij} \cdot \hat{r}_{ij} = 1$$

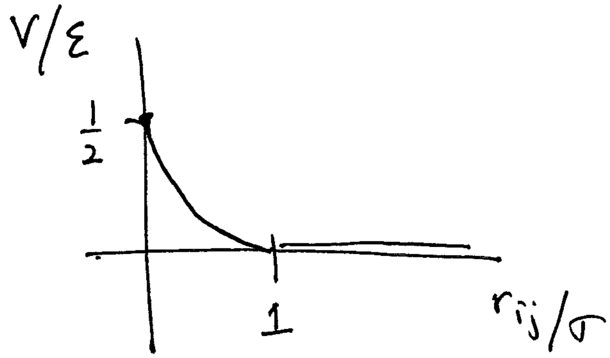


repulsive force if $\vec{F}_{ij} \propto \hat{r}_{ij}$, i.e. $F_{ij} > 0$

attractive force if $\vec{F}_{ij} \propto -\hat{r}_{ij}$, ie $F_{ij} < 0$

$$\vec{F}_i = -\vec{\nabla}_i V = -\begin{pmatrix} \frac{\partial V}{\partial x_i} \\ \frac{\partial V}{\partial y_i} \end{pmatrix}$$

$$V = \frac{\varepsilon}{2}\left(1 - \frac{r_{ij}}{\sigma}\right)^2 \theta\left(\sigma - r_{ij}\right)$$



$$\frac{\partial V}{\partial x_i} = -\frac{\varepsilon}{\sigma}\left(1 - \frac{r_{ij}}{\sigma}\right)\frac{\partial r_{ij}}{\partial x_i}$$

$$r_{ij} = \sqrt{x_{ij}^2 + y_{ij}^2} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$$

$$\frac{\partial r_{ij}}{\partial x_i} = \frac{1}{2} \cdot 2\,\frac{x_{ij}}{r_{ij}} = \frac{x_{ij}}{r_{ij}}$$

$$\frac{\partial V}{\partial x_i} = -\frac{\varepsilon}{\sigma}\left(1 - \frac{r_{ij}}{\sigma}\right)\frac{x_{ij}}{r_{ij}}$$

$$\frac{\partial V}{\partial y_i} = -\varepsilon\left(1 - \frac{r_{ij}}{\sigma}\right)\frac{y_{ij}}{r_{ij}}$$

$$\vec{F}_i = +\frac{\varepsilon}{\sigma}\begin{pmatrix} \frac{x_{ij}}{r_{ij}} \\ \frac{y_{ij}}{r_{ij}} \end{pmatrix}\left(1 - \frac{r_{ij}}{\sigma}\right)$$

$$\hat{r}_{ij} = \frac{\vec{r}_{ij}}{r_{ij}} \qquad \vec{r}_{ij} = \begin{pmatrix} x_{ij} \\ y_{ij} \end{pmatrix}$$

$$\vec{F}_i = \frac{\varepsilon}{\sigma}\left(1 - \frac{r_{ij}}{\sigma}\right)\hat{r}_{ij}$$

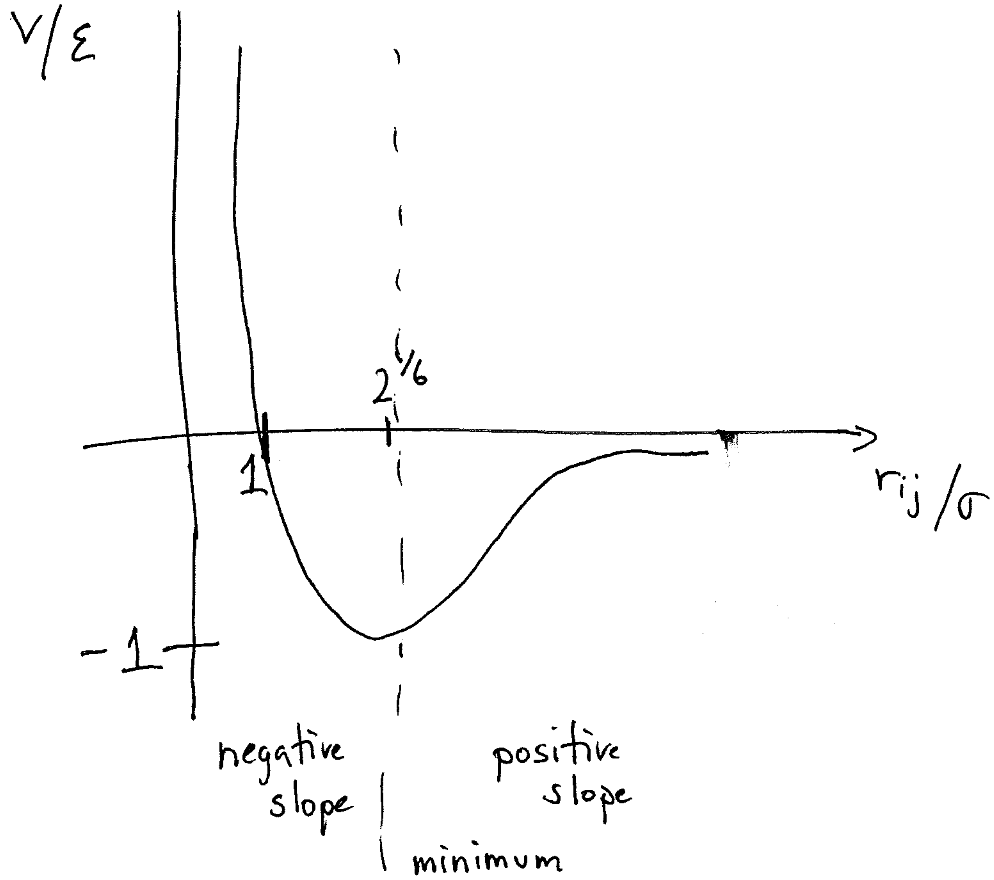
purely repulsive spring
force is repulsive,
(Potential always has
negative slope)

For central potentials, only depend on separation between particles i an j

$$\vec{F}_i = -\vec{\nabla}_i V$$

$$= -\frac{\partial V}{\partial r_{ij}}\hat{r}_{ij}$$

$$V(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$



$$\vec{F}_{ij}(r_{ij}) = -4\varepsilon\left[-12\frac{\sigma^{12}}{r_{ij}^{13}} - (-6)\frac{\sigma^6}{r_{ij}^7}\right]$$

$$= \frac{24\varepsilon}{r_{ij}}\left[2\left(\frac{\sigma}{r_{ij}}\right)^{12} - 2\left(\frac{\sigma}{r_{ij}}\right)^{6}\right] > 0$$

for $r_{ij} > 2^{1/6}\sigma$

$= \quad u(r_{ij}) = \varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - 2\left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$ for $r_{ij} < \sigma_{ij}$

$u(r_{ij}) = \left[\left(\frac{\sigma}{r_{ij}}\right)^{6} - 1\right]^{2}$

$$F(r_{ij}) = \varepsilon \; +12\left[\frac{\sigma^{12}}{r_{ij}^{13}} - 8\frac{\sigma^6}{r_{ij}^7}\right]$$

$$= \frac{6\varepsilon}{r_{ij}}\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

Numerical Integration

$$\frac{dy}{dt} = (1+y^2)\, e^t \qquad y(0) = 0$$

$$\frac{dy}{1+y^2} = e^t\, dt$$

$$\tan^{-1} y = e^t + C$$

$$y(t) = \tan\left(e^t + C\right)$$

$$y(0) = 0 \qquad C = -1$$

$$y(t) = \tan\left[e^t - 1\right] \qquad \frac{d}{du}\tan u = \frac{1}{\cos^2 u}$$

$$\frac{dy}{dt} = \frac{e^t}{\cos^2\left[e^t - 1\right]} \qquad 1 + \tan^2 x =$$

$$1 + \frac{\sin^2 x}{\cos^2 x} =$$

$$= \left(1 + \tan^2\left(e^t - 1\right)\right) e^t$$

$$\frac{dy}{dt} = (1+y^2)\, e^t \qquad \frac{1}{\cos^2 x}$$

Euler's Method

$$\boxed{\frac{dy}{dt} = f(y,t)}$$

1. Select Δt

$$\Delta t = \frac{b-a}{n} \qquad n = \frac{b-a}{\Delta t}$$

2. For $n = \dfrac{b-a}{\Delta t}$ $\qquad j = 0, 1, \ldots, n$

$$t_{j+1} = t_j + \Delta t$$

$$y(t_{j+1}) = y(t_j) + f(t_j, y_j)\Delta t$$

$$m\ddot{x}_i = F_{x_i}$$

$$\vec{F} = \frac{\varepsilon}{\sigma_{ij}}\left(1-\frac{r_{ij}}{\sigma_{ij}}\right)\hat{r}_{ij}$$

$$F_{x_i} = \frac{\varepsilon}{\sigma_{ij}}\left(1-\frac{r_{ij}}{\sigma_{ij}}\right)\frac{x_{ij}}{r_{ij}}$$

$$m\frac{\ddot{x}_i}{\sigma} = \frac{F_{x_i}}{\sigma}$$

$$= \frac{\varepsilon}{\sigma^2}\left(1-\frac{r_{ij}}{\sigma_{ij}}\right)\frac{x_{ij}/\sigma}{r_{ij}/\sigma}$$

$$m\frac{\sigma^2}{\varepsilon}\frac{\ddot{x}_i}{\sigma} = \left(1-\frac{r_{ij}}{\sigma_{ij}}\right)\frac{x_{ij}/\sigma}{r_{ij}/\sigma}$$

$$mv^2 = \varepsilon$$

$$v^2 = \frac{\varepsilon}{m}$$

$$\frac{\sigma^2}{t^2} = \frac{\varepsilon}{m}$$

$$t^2 = \sigma^2\frac{m}{\varepsilon}$$

$$t = \sigma\sqrt{\frac{m}{\varepsilon}}$$

$$\frac{m\sigma^2}{\varepsilon}\frac{d^2 x_i/\sigma}{dt^2} = \left(1-\bar{r}_{ij}\right)\frac{\bar{x}_{ij}}{\bar{r}_{ij}}$$

$$\boxed{\frac{d^2\bar{x}_i}{d\bar{t}^2} = \left(1-\bar{r}_{ij}\right)\frac{\bar{x}_{ij}}{\bar{r}_{ij}}}$$

$$\bar{t} = \frac{\cancel{\sigma}}{\cancel{\sqrt{\varepsilon/m}}} = \frac{t}{\sigma\sqrt{\frac{m}{\varepsilon}}}$$