1

$$m\ddot{x}_i = F_i(x_j)$$

$$m(\dot{v}_i) = F_i(x_j)$$

(any coord. w/o time superscript is at t)

$$m\left(\frac{v_i^{t+dt} - v_i^{t}}{dt}\right) = F_i$$

$$\Rightarrow \quad v_i^{t+dt} = v_i^{t} + \frac{F}{m_i}\cdot dt$$

$$\dot{x}_i = v_i = \frac{x_i^{t+dt} - x_i^{t}}{dt}$$

$$\Rightarrow \quad x_i^{t+dt} = x_i^{t} + v_i^{t}\, dt$$

algorithm:

set x_i^0, v_i^0 $\quad \forall i$; specify dt

set $t_1 = 0$

$\rightarrow t_2 = t_1 + dt$

calc. $\quad x_i^{t_2} = x_i^{t_1} + v_i^{t_1}\, dt \quad \forall i$

$$v_i^{t_2} = v_i^{t_1} + \frac{F(x_j^{t_1}, v_j^{t_1})}{m_i}\, dt$$

set $t_1 = t_2$

what do I want F to look like?

parameters

i. 3d Box with center at coord. origin $(0,0)$ — box size a

ii. (weak) gravitational pull towards the center — strength $-\frac{m_i k \binom{x_i}{y_i}}{(x_i^2+y_i^2)^{3/2}} \mathrel{\hat{=}} -\frac{Gm\vec{r}}{|\vec{r}|^3}$

iii. inter particle, short-range attraction/repulsion — range/strength $c\cdot\exp\left(-\alpha\left((x_i-x_j)^2 + (y_i-y_j)^2\right)\right)$

~~grad~~ potential

"Gaussian Force" for particle i

$$-2\alpha(\vec{r}_n - \vec{r}_j)\sum_{j\neq i} e^{-\alpha\Delta r_j^2} = -2\alpha \sum_{j\neq i} \binom{x_n - x_j}{y_n - y_j} e^{-\alpha(\vec{r}_n - \vec{r}_j)^2}$$

2

$$P_i^{box} = \frac{1}{\exp\left[\frac{r_i - \mu}{k}\right] + 1}$$

"Fermi" box

$$r_i^t \equiv \left({x_i^t}^2 + {y_i^t}^2 \right)^{1/2}$$

$$\Rightarrow \quad f_i^{box} = \vec{\nabla} P_i^{box}$$

x - compo:

$$\partial_{x_i} \frac{1}{e^{k^{-1}(\sqrt{x_i^2+y_i^2} - \mu)} + 1} = \frac{-1}{\left(e^{k^{-1}(r-\mu)} + 1\right)^2} \cdot \left(k^{-1} \frac{1}{r} \cdot \frac{1}{2} \cdot 2x_i \right)$$

$$= -\frac{x_i}{kr} \frac{1}{(\ldots)^2}$$

$\Rightarrow$ we need to implement

$$f_i^{grav} = -\frac{m_i G}{|\vec{r}_i|^3} \cdot \vec{r}_i$$

$$f_i^{short} = -2\alpha \sum_{j \neq i} (\vec{r}_i - \vec{r}_j)\, e^{-\alpha(\vec{r}_i - \vec{r}_j)^2}$$

$$f_i^{box} = -\frac{\vec{r}_i}{k|\vec{r}_i|} \left(\exp\left[\frac{|\vec{r}| - \mu}{k}\right] + 1 \right)^{-2}$$

$$\vec{r}_i = \begin{pmatrix} x_i^t \\ y_i^t \end{pmatrix}$$