Partikel Simulation Notizen von

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Eigene Definitionen Basis-Variablen

- $p \rightarrow$ liste aller Partikel
- $i \rightarrow$ Partikel i
- $j \rightarrow$ Partikel j
- $x \rightarrow$ Position
- $v \rightarrow$ Geschwindigkeit
- $a \rightarrow$ Beschleunigung
- $m \rightarrow$ Masse
- $n \rightarrow$ Zeitschrittnummer
- $\Delta t \rightarrow$ Zeitschrittgröße
- $\sigma \rightarrow$???
- $\epsilon \rightarrow$???

Eigene Definitionen Initialisierungen

$$\vec{x_0} = random \tag{1}$$
$$\vec{v_0} = \vec{0} \tag{2}$$
$$\vec{a_0} = \vec{0} \tag{3}$$
$$\sigma = 1 \tag{4}$$
$$\epsilon = 1 \tag{5}$$
$$A_{i,j} = 48\epsilon_{i,j}\sigma_{i,j}^{12}\Delta t^2 \tag{6}$$
$$B_{i,j} = 24\epsilon_{i,j}\sigma_{i,j}^{6}\Delta t^2 \tag{7}$$
$$s_{n,i,j} = \frac{A_{i,j} - B_{i,j}r_{n,i,j}^6}{r_{n,i,j}^{14}} \tag{8}$$
$$\vec{d}_{n,i,j} = \vec{x}_{n,j} - \vec{x}_{n,i} \tag{9}$$
$$r_{n,i,j} = \left\|\vec{d}_{n,i,j}\right\| \tag{10}$$
$$\tag{11}$$

Lennard Jones

Siehe Rapport The Art of Molecular Dynamics Simulation Seite 12 unten.

$$f_{n,i,j} = \left(\frac{48\epsilon_{i,j}}{\sigma_{i,j}^2}\right)\left[\left(\frac{\sigma_{i,j}}{r_{n,i,j}}\right)^{14} - \frac{1}{2}\left(\frac{\sigma_{i,j}}{r_{n,i,j}}\right)^{8}\right] r_{n,i,j}$$

Verlet Algorithmus

Siehe Wikipedia `https://de.wikipedia.org/wiki/Verlet-Algorithmus`

$$\vec{x}_{1,i} = \vec{x}_{0,i} + \vec{v}_{0,i}\Delta t + \frac{1}{2}\vec{a}_{0,i}\Delta t^2$$
$$\vec{x}_{n+1,i} = 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \vec{a}_{n,i}\Delta t^2$$

Kraft ↔ Beschleunigung

$$f = ma$$
$$a = \frac{f}{m}$$

gerichtete Kraft von i nach j

$$\vec{a}_{n,i,j} = \frac{a_{n,i,j}}{r_{n,i,j}}\left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)$$

Alles Zusammen

$$\vec{x}_{n+1,i} = 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \vec{a}_{n,i,j}\Delta t^2 \tag{12}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in p\wedge i\neq j} \frac{a_{n,i,j}}{r_{n,i,j}} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)\Delta t^2 \tag{13}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{\frac{f_{n,i,j}}{m_i}}{r_{n,i,j}} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)\Delta t^2 \tag{14}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{f_{n,i,j}}{m_i r_{n,i,j}} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)\Delta t^2 \tag{15}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{\left(\frac{48\epsilon_{i,j}}{\sigma_{i,j}^2}\right)\left[\left(\frac{\sigma_{i,j}}{r_{n,i,j}}\right)^{14} - \frac{1}{2}\left(\frac{\sigma_{i,j}}{r_{n,i,j}}\right)^{8}\right] r_{n,i,j}}{m_i r_{n,i,j}} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)\Delta t^2 \tag{16}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{\left(\frac{48\epsilon_{i,j}}{\sigma_{i,j}^2}\right)\left[\left(\frac{\sigma_{i,j}}{r_{n,i,j}}\right)^{14} - \frac{1}{2}\left(\frac{\sigma_{i,j}}{r_{n,i,j}}\right)^{8}\right]}{m_i} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)\Delta t^2 \tag{17}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{\left(\frac{48\epsilon_{i,j}}{\sigma_{i,j}^2}\right)\left[\left(\frac{\sigma_{i,j}^{14}}{r_{n,i,j}^{14}}\right) - \frac{1}{2}\left(\frac{\sigma_{i,j}^{8}}{r_{n,i,j}^{8}}\right)\right]}{m_i} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)\Delta t^2 \tag{18}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{\left(48\epsilon_{i,j}\sigma_{i,j}^6\right)\left[\left(\frac{\sigma_{i,j}^{6}}{r_{n,i,j}^{14}}\right) - \left(\frac{0.5}{r_{n,i,j}^{8}}\right)\right]}{m_i} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)\Delta t^2 \tag{19}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{\left(48\epsilon_{i,j}\sigma_{i,j}^6\right)\left[\left(\frac{\sigma_{i,j}^{6}}{r_{n,i,j}^{14}}\right) - \left(\frac{0.5r_{n,i,j}^{6}}{r_{n,i,j}^{14}}\right)\right]}{m_i} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)\Delta t^2 \tag{20}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{\left(48\epsilon_{i,j}\sigma_{i,j}^6\right)\left[\frac{\sigma_{i,j}^{6} - 0.5r_{n,i,j}^{6}}{r_{n,i,j}^{14}}\right]}{m_i} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)\Delta t^2 \tag{21}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{\frac{48\epsilon_{i,j}\sigma_{i,j}^6\sigma_{i,j}^6 - 24\epsilon_{i,j}\sigma_{i,j}^6 r_{n,i,j}^6}{r_{n,i,j}^{14}}}{m_i} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)\Delta t^2 \tag{22}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{48\epsilon_{i,j}\sigma_{i,j}^{12} - 24\epsilon_{i,j}\sigma_{i,j}^6 r_{n,i,j}^6}{r_{n,i,j}^{14} m_i} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right)\Delta t^2 \tag{23}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{A_{i,j} - B_{i,j} r_{n,i,j}^6}{r_{n,i,j}^{14} m_i} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right) \tag{24}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{s_{n,i,j}}{m_i} \left(\vec{x}_{n,j} - \vec{x}_{n,i}\right) \tag{25}$$

$$= 2\vec{x}_{n,i} - \vec{x}_{n-1,i} + \sum_{j\in(p\setminus i)} \frac{s_{n,i,j}}{m_i} \vec{d}_{n,i,j} \tag{26}$$

$$\tag{27}$$