DKRZ
DEUTSCHES KLIMARECHENZENTRUM

Veranstaltung: _____

Name: _____ Datum: _____

N

$\vec{x}_i, \vec{v}_i, \vec{F}_i$

$\rightarrow \frac{d\vec{v}_i(t)}{dt} = \vec{v}_i$

$m \frac{d\vec{v}_i}{dt} = \vec{F}_i = \sum_{j \neq i} \vec{F}_{ij}$

Lennard-Jones Potential

$r_{ij} := \| \vec{x}_i - \vec{x}_j \| = \sqrt{\sum_{d} (x_i - x_j)^2_d}$

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

$F_{ij} = -\nabla U$

$\varepsilon = \sqrt{\varepsilon_1 \varepsilon_2}$, $\frac{\sigma_1 + \sigma_2}{2} = \sigma_{12}$

$\frac{df}{dx}$

$x(t) = a\,x + t$

$\frac{dy}{dx} = h$

$\frac{dy}{dx} = \lim_{h \to 0} \frac{y(x+h) - y(x)}{h}$

$\approx \frac{y(x+\Delta x) - y(x)}{\Delta x}$

Δx klein

$\frac{dx_i}{dt} = v_i$

$\frac{x_i(t+\Delta t) - x_i(t)}{\Delta t} \approx v_i(t)$

$x_i(t+\Delta t) \approx x_i(t) + \Delta t\, v_i(t)$

Explizites Euler (1)

Störmer-Verlet

$m_i \frac{d^2 \vec{x}_i}{dt^2} = \vec{F}_i$

(1)

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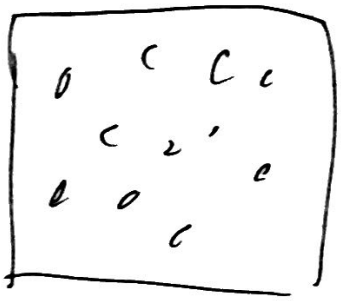
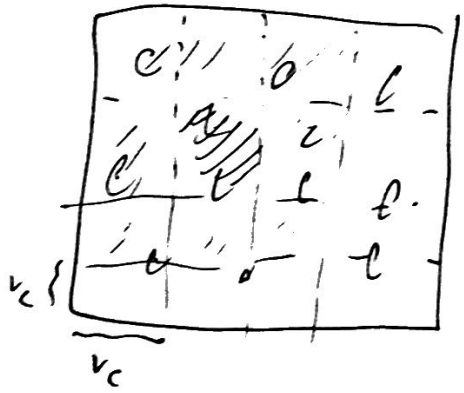


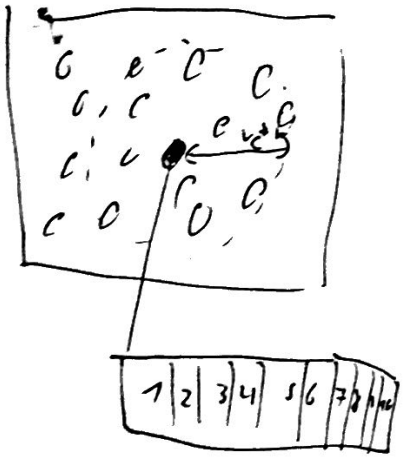
Algo:
1. Finde Partikelpaare, die nahe sind
2. Rechne Kräfte für diese Paare aus

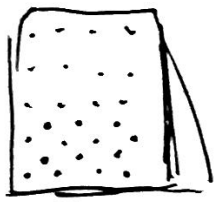
$\|x_i - x_j\| < r_c$ cut-off radius

Linked Cell



Verlet Listen





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Simulation LAMMPS, espresso, GROMACS

Visualisierung VMD, ParaView/vtk