PSE Molekulardynamik - Entwicklung eines Molekulardynamik-Simulators

Molekulardynamik-Simulation: Anwendungen

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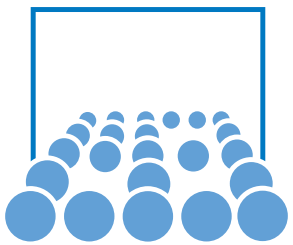
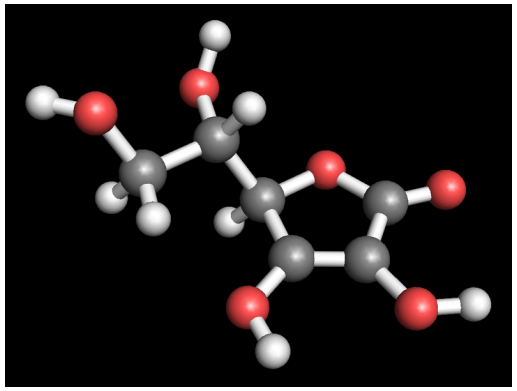


Übersicht

Application 1: Simulation of a Membrane

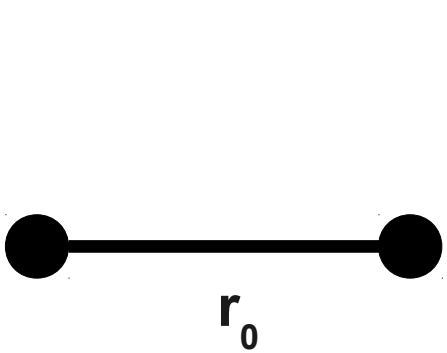
Application 2: Crystallisation of Argon

Simulation of membranes - Internal Degrees of freedom

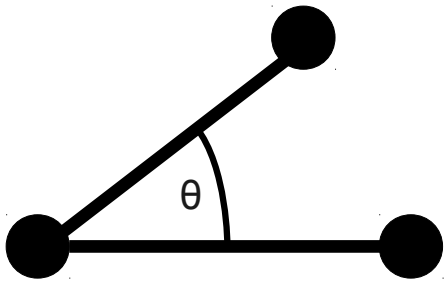


Ascorbic acid (Source: Wikipedia.de).

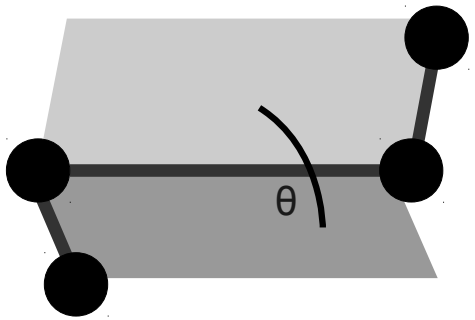
- Treat single atoms / groups of atoms individually.
- Define fixed neighbouring atoms.
- Interaction of neighbours takes place through



$$U(r_{ij}) = \frac{1}{2} k \left(r_{ij} - r_0\right)^2$$



$$U(\theta) = \frac{1}{2} k_\theta \left(\theta - \theta_0\right)^2$$



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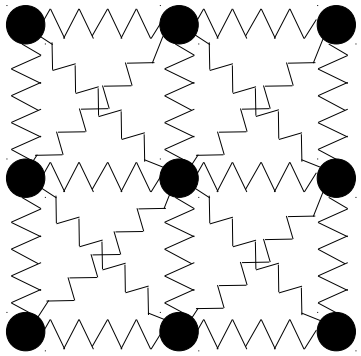
- initial setup:



- Force calculation for direct neighbours:

$$F(r_{ij}) = k \cdot (r - r_0)$$

  Force calculation for diagonal neighbours:

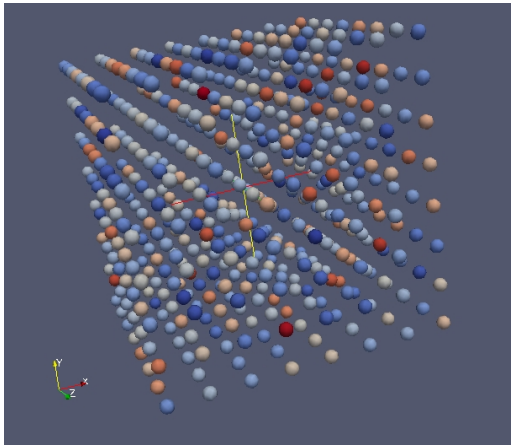
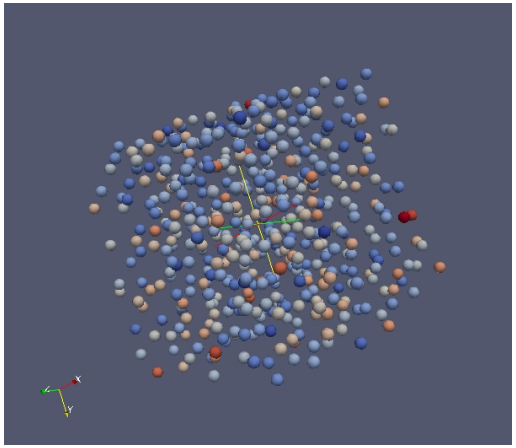
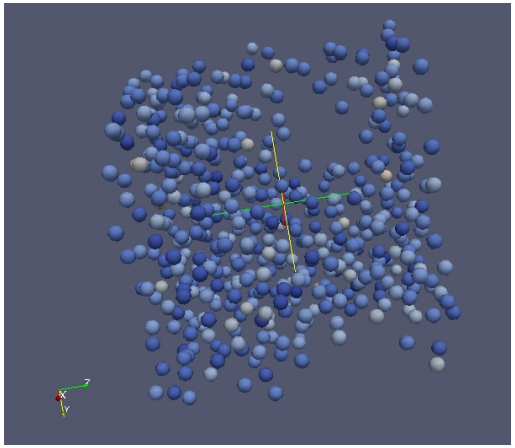
$$F(r_{ij}) = k \cdot (r - \sqrt{2} r_0)$$

- Non-neighbouring atoms: Lennard-Jones potential, truncated at $2^{\frac{1}{6}} \cdot \sigma$.

Possible further experiments:

- Nanotube, subject to gravity (or not)
- Nanotube with stretched ends (see Griebel book)
- flow of liquid / object hitting membrane
- ...

Application 2: Crystallisation of Argon

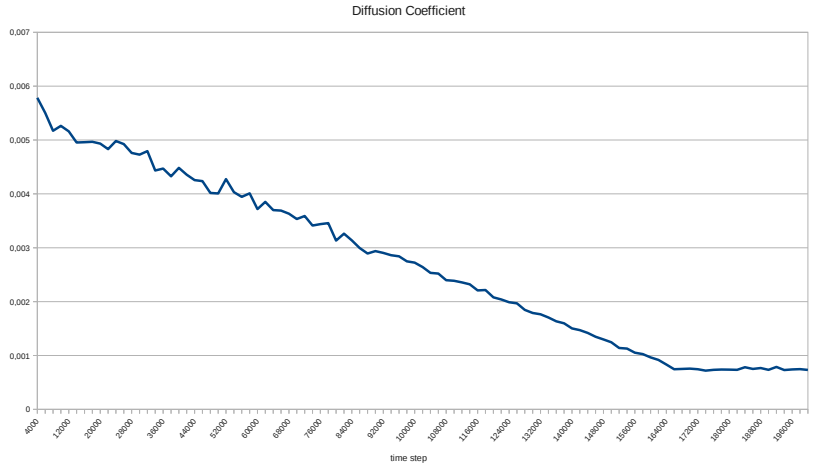




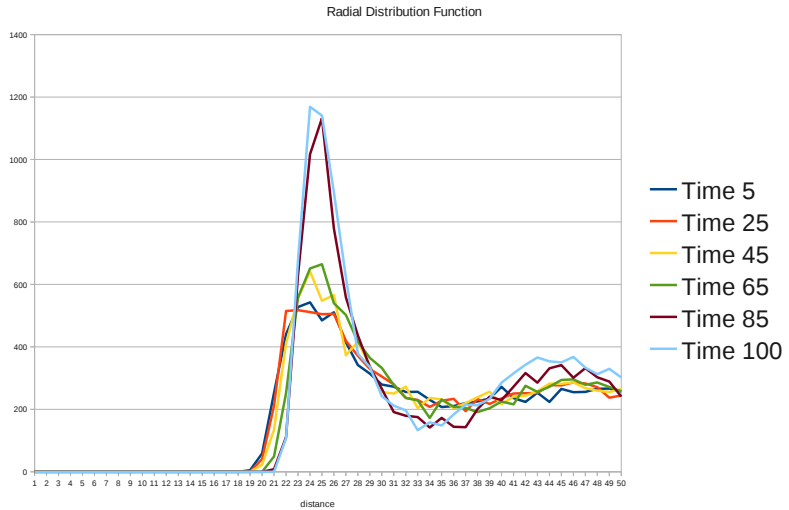
- Slow cooling: crystallisation
- Supercooling: amorphous glass state

How do you detect the aggregate state of a fluid?

- Diffusion:
  Movement of a particle during time $t - t_0$, averaged over all particles (and several time steps):

$$Var(t) = \frac{1}{N} \sum_{i=1}^{N} \| x_i(t) - x_i(t_0) \|^2$$





- Radial Pair Distribution Function - RDF:
  Describes the Probability to find a molecule in the neighbourhood of another molecule at distance r.
  Calculation:
  - Discretize distance $0 \leq r < r_{cutoff}$ in intervalls of length δr:
  - Count molecule pairs with distance $r \in]r_i; r_i + \delta r]$.
  - Compute local density by dividing the above number by the volume of the $\frac{4\pi}{3}\left((r_i + \delta r)^3 - r_i^3\right)$ geteilt wird.

- Potential Energy / Pressure