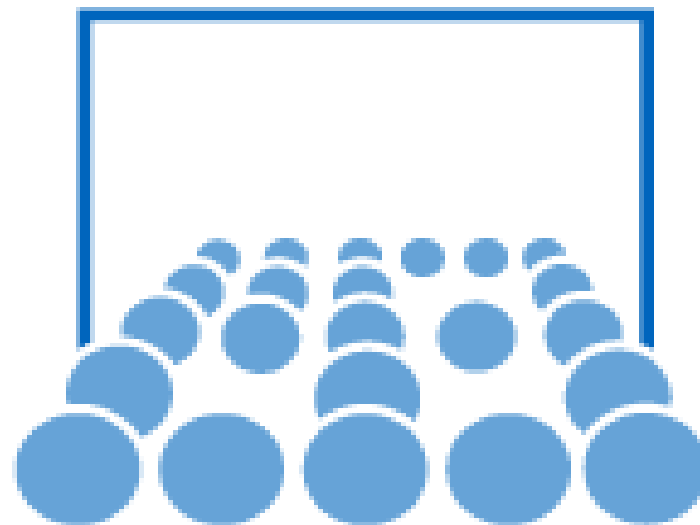


PSE Molekulardynamik

MD-basics,
Unit tests & Assertions

Alexander Breuer, Benjamin Uekermann

24.10.2014



Outline

- Schedule
- Presentations: Worksheet 1
- Lennard-Jones potential & Brownian motion
- Assertions & Unit tests
- Preparation: Worksheet 2

Schedule

10.10.2014	Intro 1 WS
24.10.2014	Review 1 WS / Intro 2 WS
07.11.2014	Review 2 WS / Intro 3 WS
28.11.2014	Review 3 WS / Intro 4 WS
12.12.2014	Review 4 WS / Intro 5 WS
16.01.2015	Review 5 WS

Presentations: Worksheet 1

Lennard-Jones potential

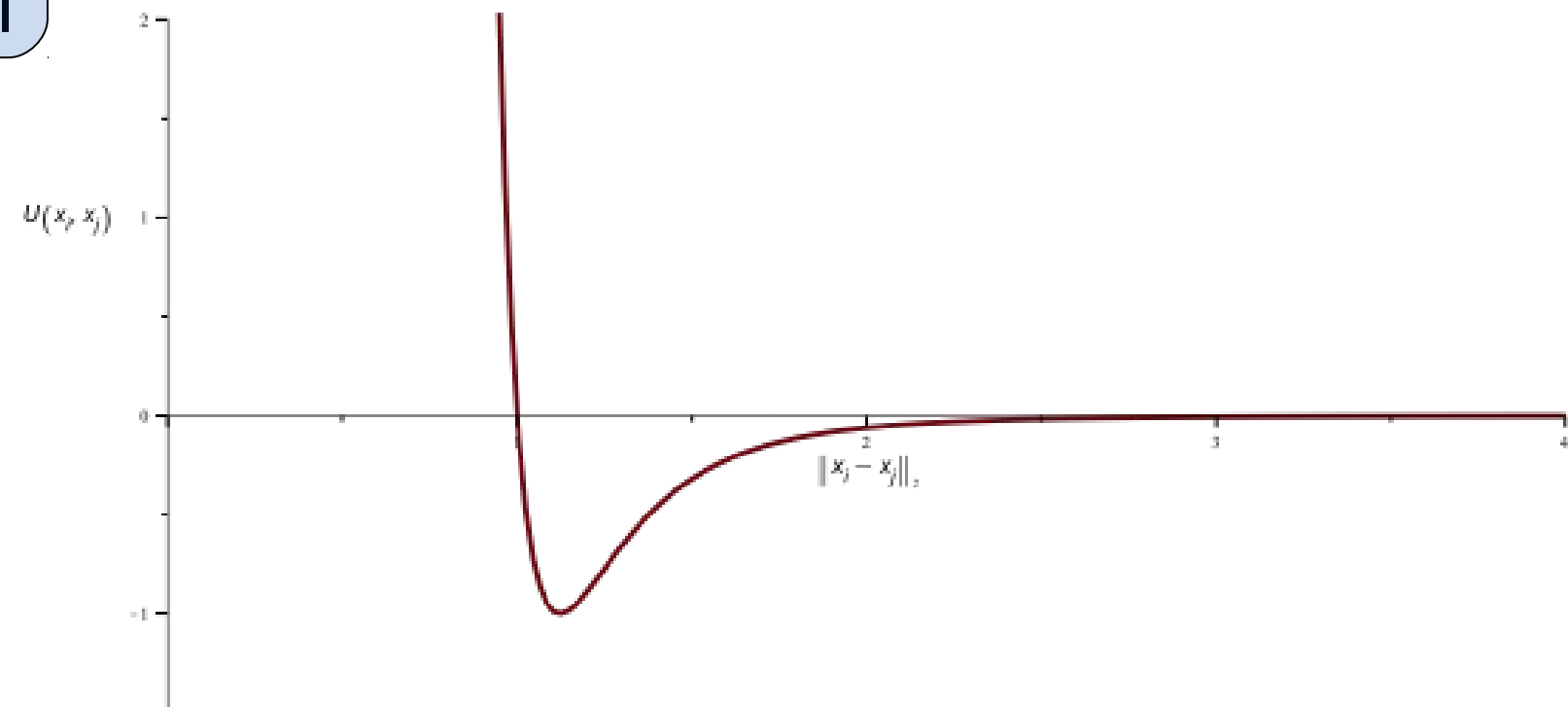
- Interaction between molecules or atoms

$$U(\mathbf{x}_i, \mathbf{x}_j) = 4\epsilon \left(\left(\frac{\sigma}{\|\mathbf{x}_i - \mathbf{x}_j\|_2} \right)^{12} - \left(\frac{\sigma}{\|\mathbf{x}_i - \mathbf{x}_j\|_2} \right)^6 \right)$$

potential well

solidity

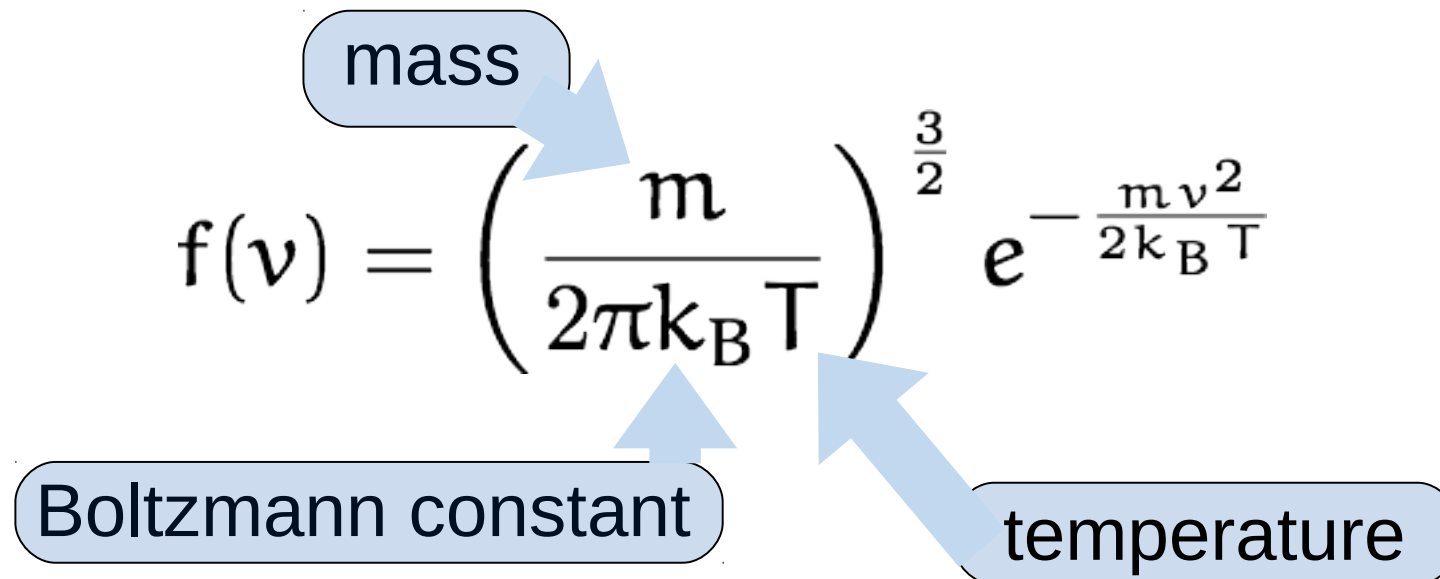
zero-crossing



Lennard-Jones potential
for $\epsilon = 1$ and $\sigma = 1$

Brownian Motion

- Temperature \Rightarrow random movement of particles
- Implementation: Maxwell-Boltzmann distribution

$$f(\mathbf{v}) = \left(\frac{m}{2\pi k_B T} \right)^{\frac{3}{2}} e^{-\frac{m v^2}{2k_B T}}$$


The diagram illustrates the Maxwell-Boltzmann distribution equation. Three blue arrows point from labels in rounded rectangular boxes to the corresponding variables in the equation: 'mass' points to 'm', 'Boltzmann constant' points to 'k_B', and 'temperature' points to 'T'.

- Sheet 2: Code @ homepage Sheet 2: 2D-functionality of the function

Preparation: Worksheet 2