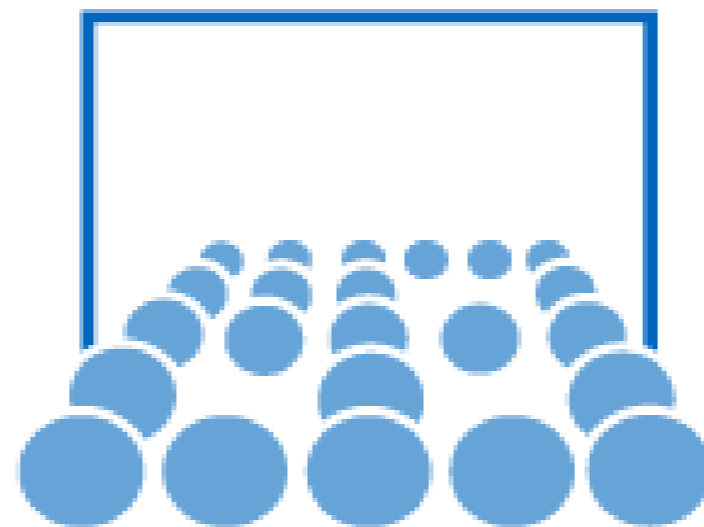


PSE Molekulardynamik

MD-basics,
Unit tests & Assertions

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30.10.2015



Outline

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

Schedule (big meetings)

16.10.2015	Intro 1 WS
30.10.2015	Review 1 WS / Intro 2 WS
13.11.2015	Review 2 WS / Intro 3 WS
04.12.2015	Review 3 WS / Intro 4 WS
18.12.2015	Review 4 WS / Intro 5 WS
16.01.2016	Review 5 WS

Presentations: Worksheet 1

Lennard-Jones potential

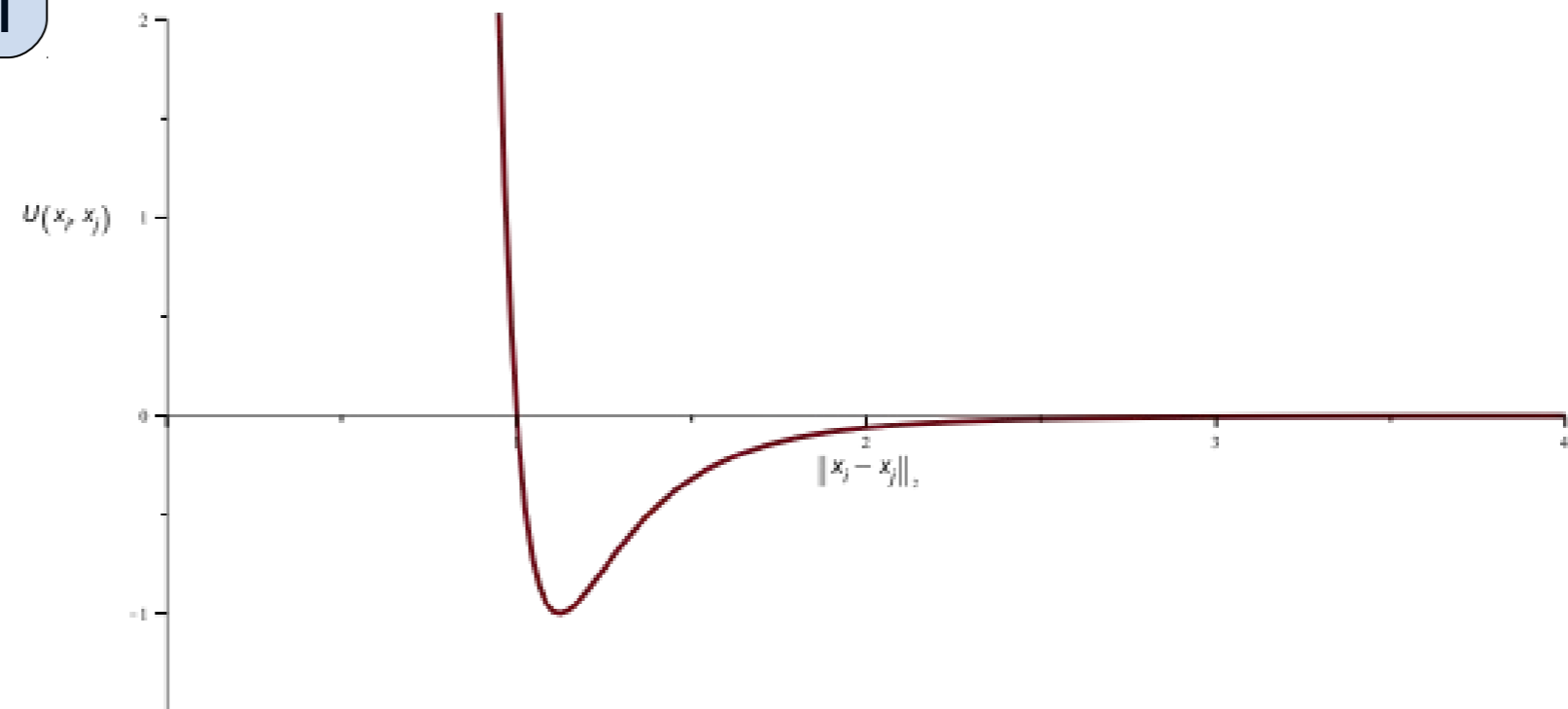
- Interaction between molecules or atoms

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

potential well

solidity

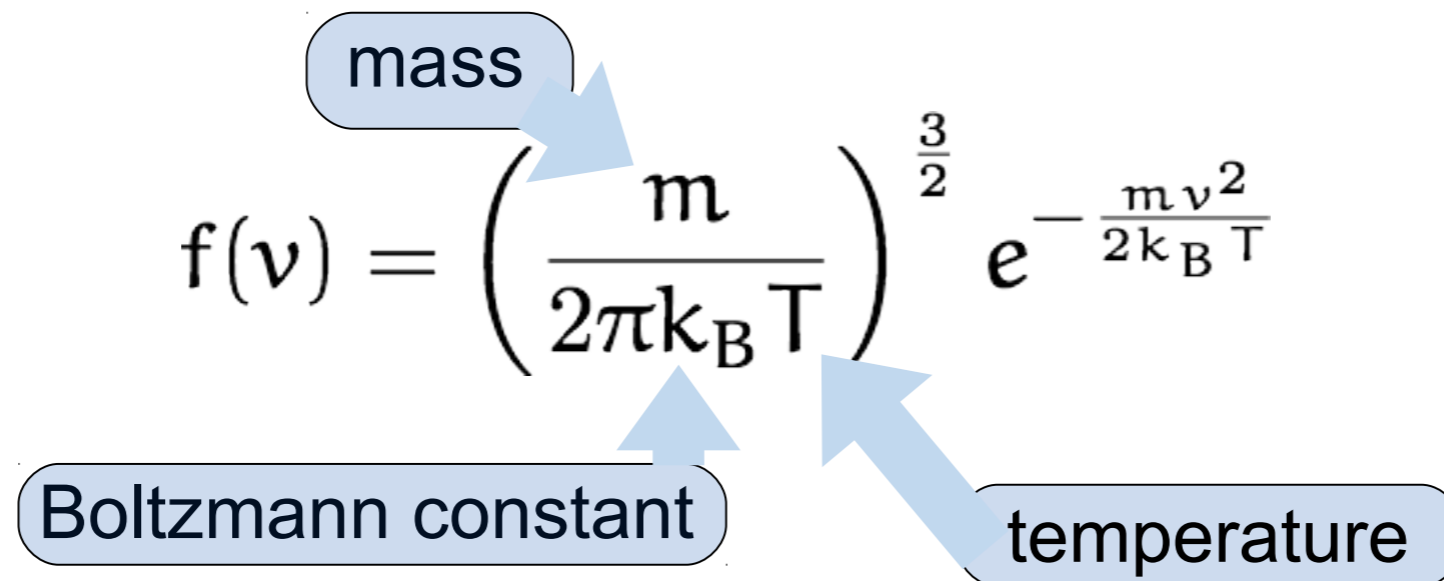
zero-crossing



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

Brownian Motion

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

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


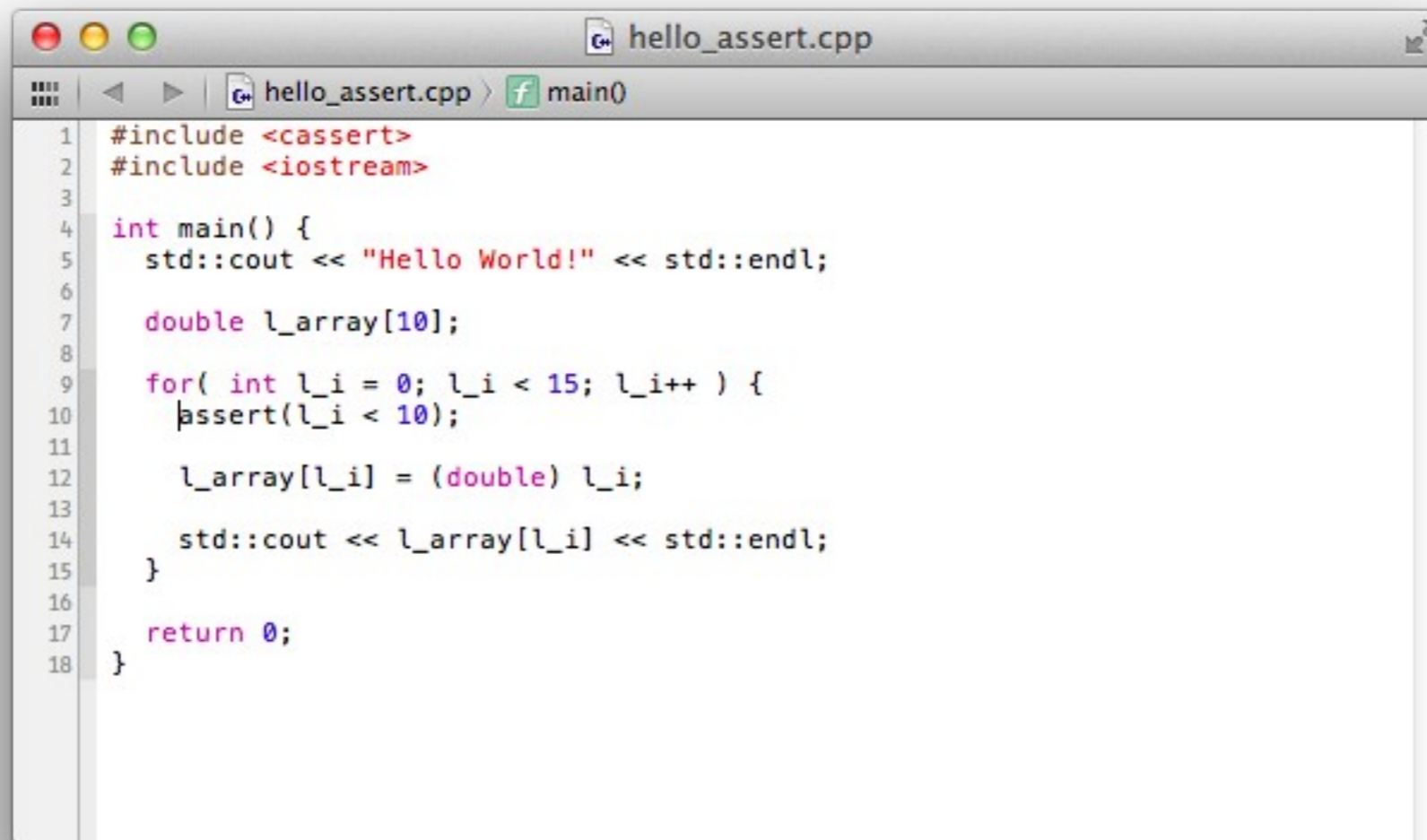
The diagram illustrates the Maxwell-Boltzmann distribution equation. Three callout boxes with arrows point to specific parts of the equation: 'mass' points to the 'm' in the numerator of the fraction; 'Boltzmann constant' points to the 'k_B' in the denominator; and 'temperature' points to the 'T' in the denominator.

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

Preparation: Worksheet 2

Assertions

- Example: Hello world



```
hello_assert.cpp
main()
1 #include <cassert>
2 #include <iostream>
3
4 int main() {
5     std::cout << "Hello World!" << std::endl;
6
7     double l_array[10];
8
9     for( int l_i = 0; l_i < 15; l_i++ ) {
10        assert(l_i < 10);
11
12        l_array[l_i] = (double) l_i;
13
14        std::cout << l_array[l_i] << std::endl;
15    }
16
17    return 0;
18 }
```