



### Main Tasks:

- include googletest, spdlog
- add CI pipeline
- new way of calculating forces
- performance measurement
- reading files with cuboids and creating the particles accordingly
- the actual simulation

# <u>Lennard-Jones-Potential</u> using some **≥=**:-)



- calculateF() takes function parameter for force calculations between two Particles
- possible to dynamically switch between the two force calculations
- "curried" Function for Lennard-Jones-Potential

forceLennJonesPotentialFunction(double sigma, double epsilon)

$$-\frac{24 \cdot \epsilon}{(||x_i - x_j||_2)^2} \left( \left( \frac{\sigma}{||x_i - x_j||_2} \right)^6 - 2 \left( \frac{\sigma}{||x_i - x_j||_2} \right)^{12} \right) (x_i - x_j)$$

$$\frac{m_i \cdot m_j}{(\|x_i - x_j\|)^3} (x_j - x_i)$$

## <u>Performance</u>



#### Parameters:

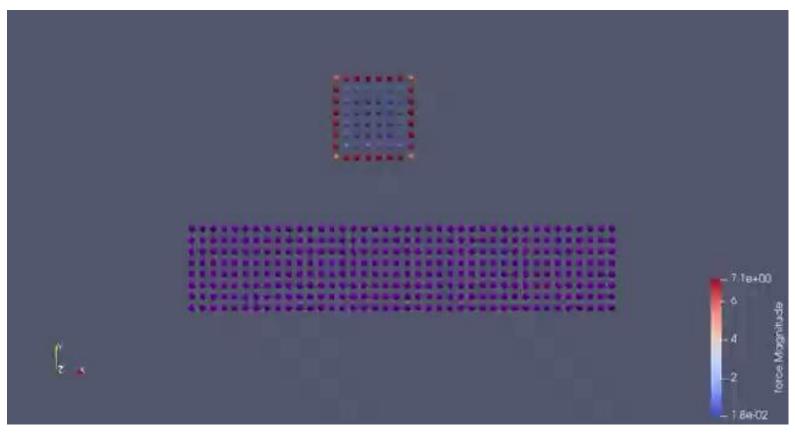
- std::chrono::high resolution clock used for time measurement
- Measurements in Linux environment on AMD Ryzen 7 5700U
- Compiled with gcc and flag -O2 for runtime measurement
- Memory access measured with cachegrind (program compiled with -O1)

	nested loop	Newtons third law
runtime	~ 122 sec	~ 114 sec
memory access	~ 5,86 bil. data accesses	~ 3,27 bil. data accesses
cache miss rate	0.1 %	0.1 %

PSE Molecular Dynamics | Groupe B | Sheet 2



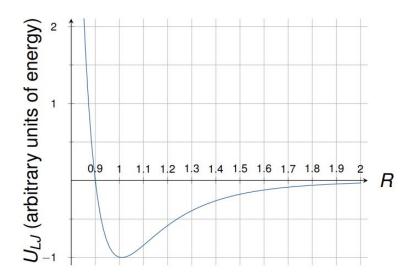




### **Observations**

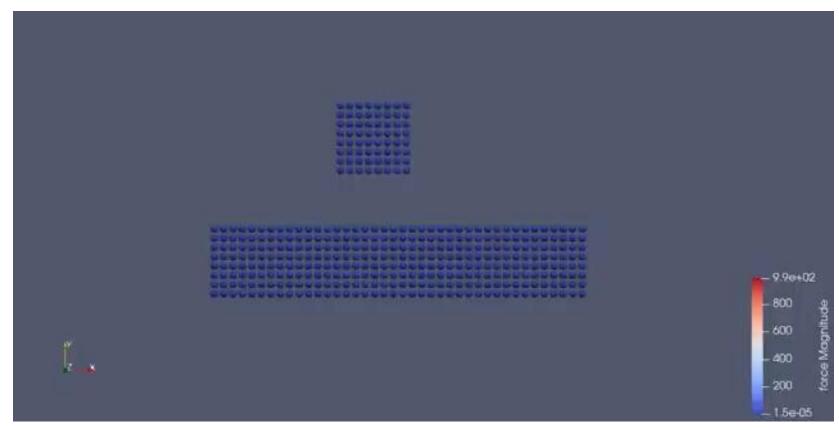


- particles push each other during collision
- force of isolated particles oscillates



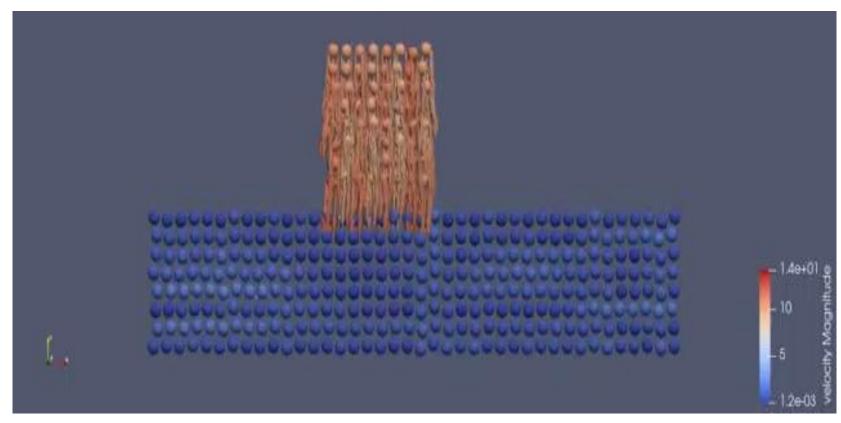










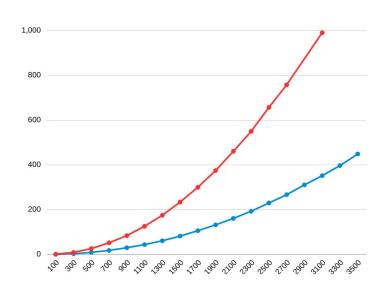


## Calculating force



- utilising Newton's third law  $F_{ij}=-F_{ji}$
- only half of the particle combinations needed

Р	0	1	2	3	4	5
0	x	~	~	~	~	~
1	~	x				
2	~		x			
3	V			х		
4	V				х	
5	V					х







- amount of force calculations non-linear

cuboid:  $20 \times 40 \times 4 = 3200 \implies 5.1 \text{ mio}$ 

cuboid:  $20 \times 35 \times 4 = 2800 \implies 3.9 \text{ mio}$ 

⇒ handshake problem

