MolSim WS 23/24

Sheet 2

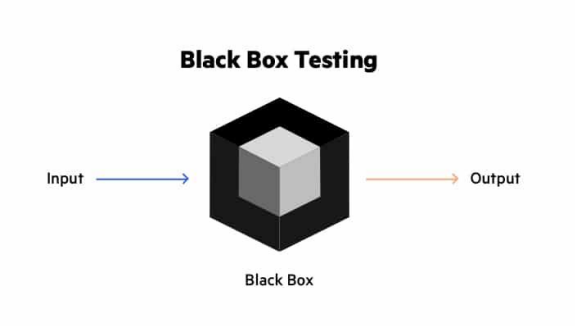
Collision of two bodies

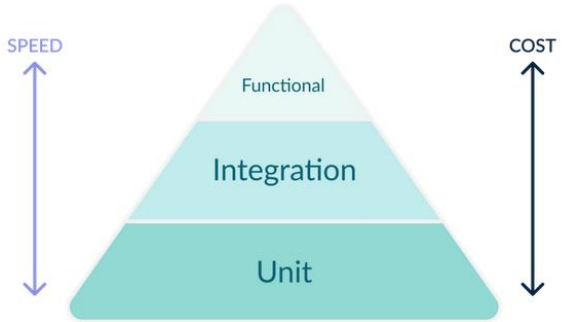
Group C [Manuel, Tobias, Daniel]

11/17/2023

Unit tests

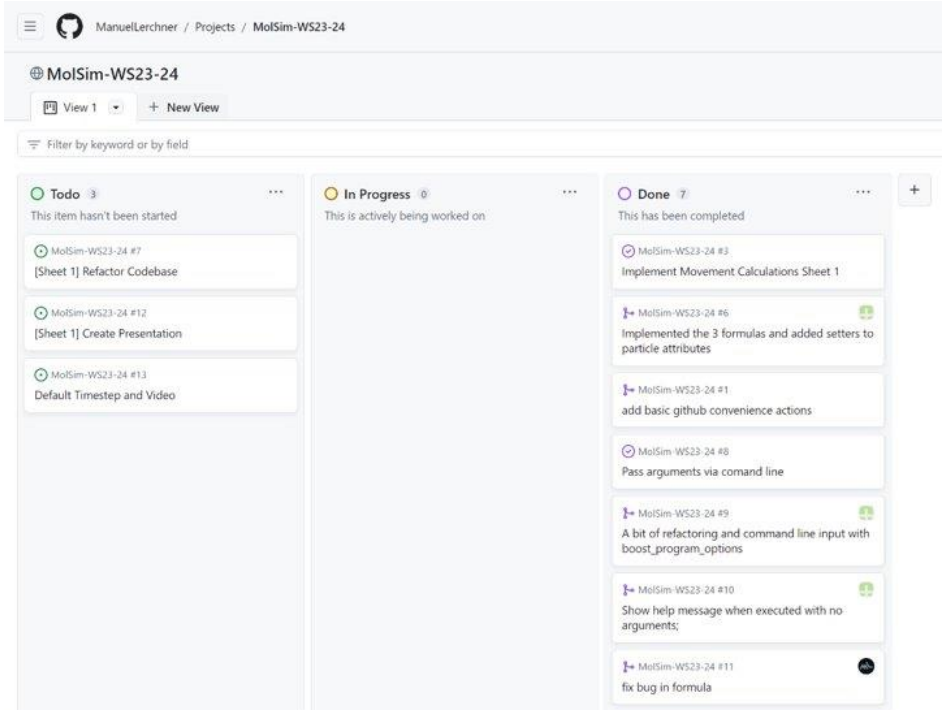
- **Important testing principles**
  - independent components
  - independent parameters
- **Different testing goals**
  - Components vs (Sub-)Systems
  - Functionality vs format





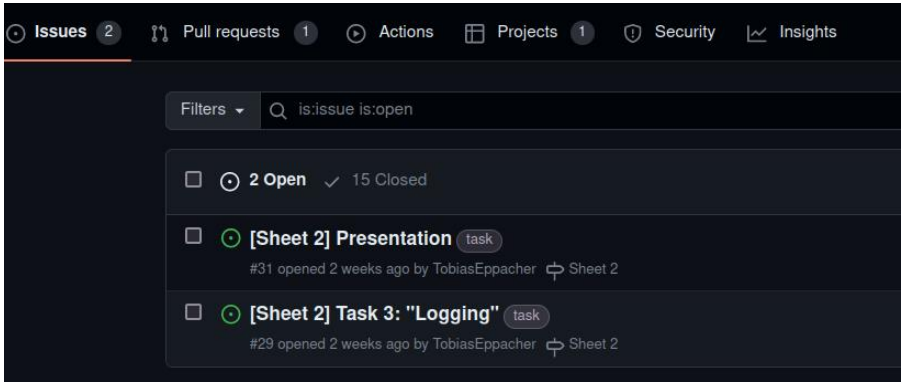
Github Project Management

- Task Planning via Github
- Kanban Board View
- Easy way to see open issues



Github Issues

- We organize open tasks in issues
- Issues can be assigned to persons
- Everyone can work in parallel
- Hopefully not many merge conflicts
- Creation of pull requests to protect the master branch



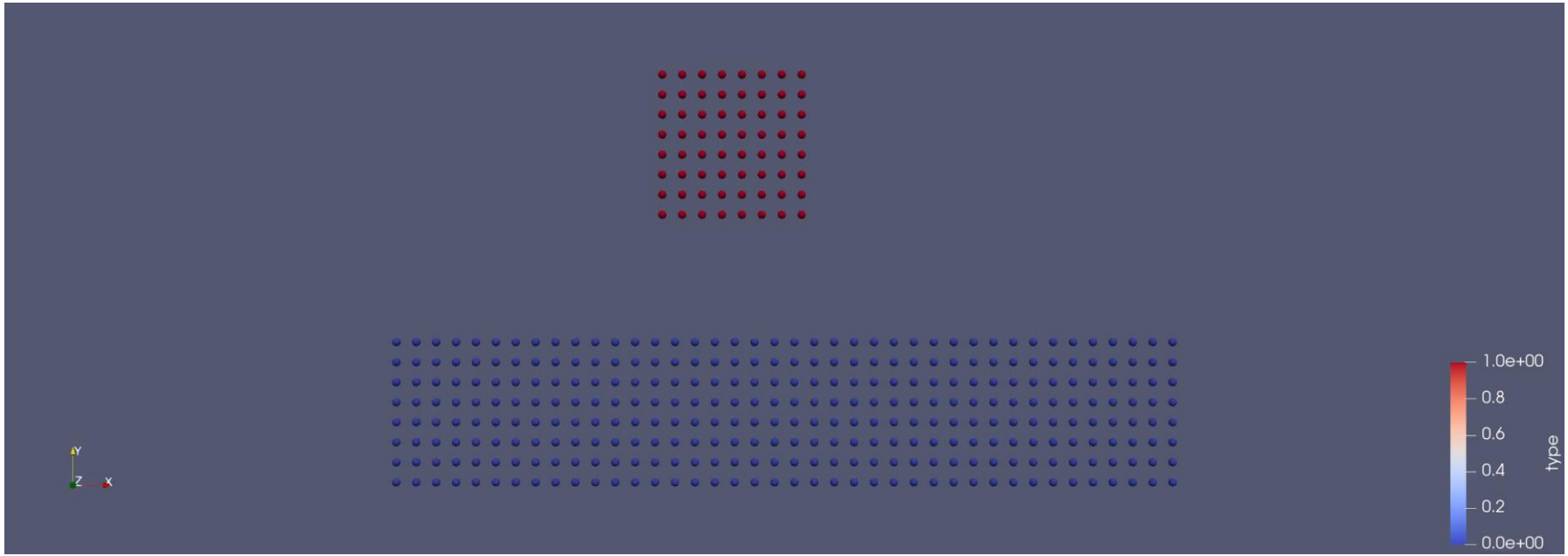
Logging

Integration of the spdlog library
Pret
Use

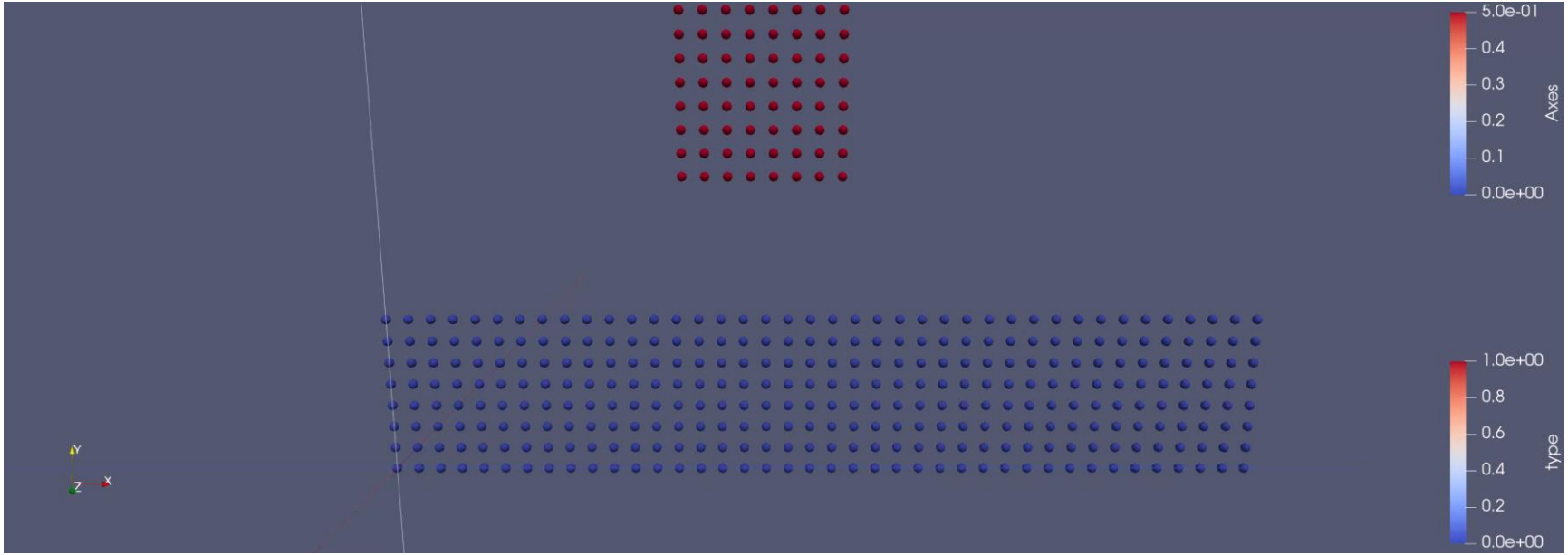
```
[18:49:54] [info] Simulation arguments:
[18:49:54] [info] Input file path: ../../input/body_collision.cub
[18:49:54] [info] Output directory path: ./output/body_collision/
[18:49:54] [info] End time: 5
[18:49:54] [info] Frames per second: 24
[18:49:54] [info] Video length: 30
[18:49:54] [info] Log level: info

[18:49:54] [error] Invalid entry in file '../../input/body_collision.cub' on line 3.
         Comments must start with: '#', but got: 's'
         Content of line: '40 8 1s              # grid dimensions'
[18:49:54] [error] Make sure that comments start after the arguments in the line.
[18:49:54] [critical] Program terminated after throwing an instance of 'FileReader::FileFormatException'.
```

Simulation 1



Simulation 1



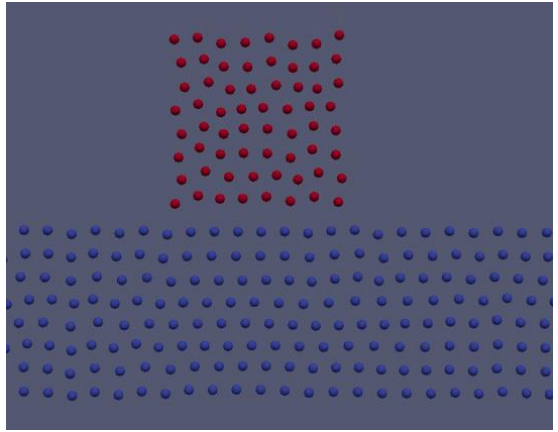
Simulation 1

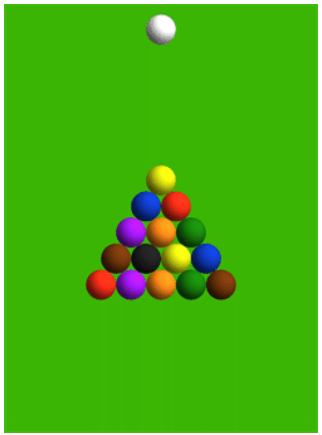
Observation 1:

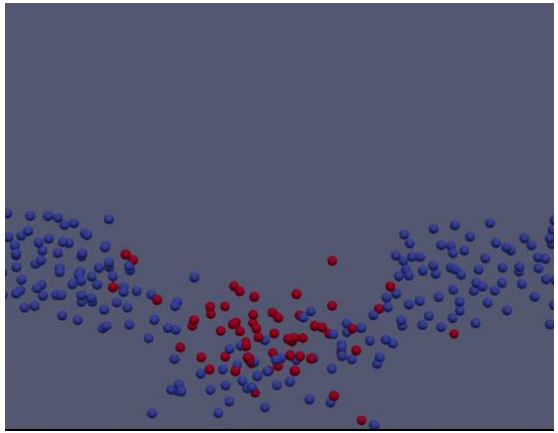
- Particles scatter on impact
- Red particles transfer momentum to a few of the blue ones
- Particles move together according to newtons 1st law

Similar processes:

- Billiard ball colliding







Simulation 1 + 2

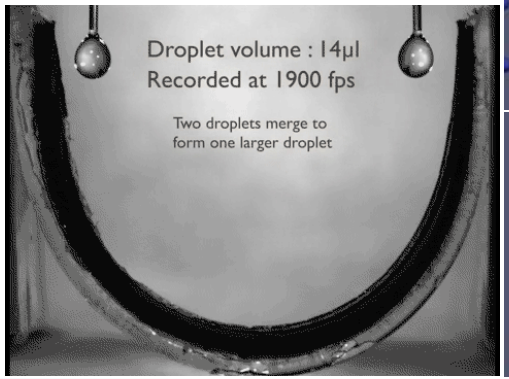
Observation 2:

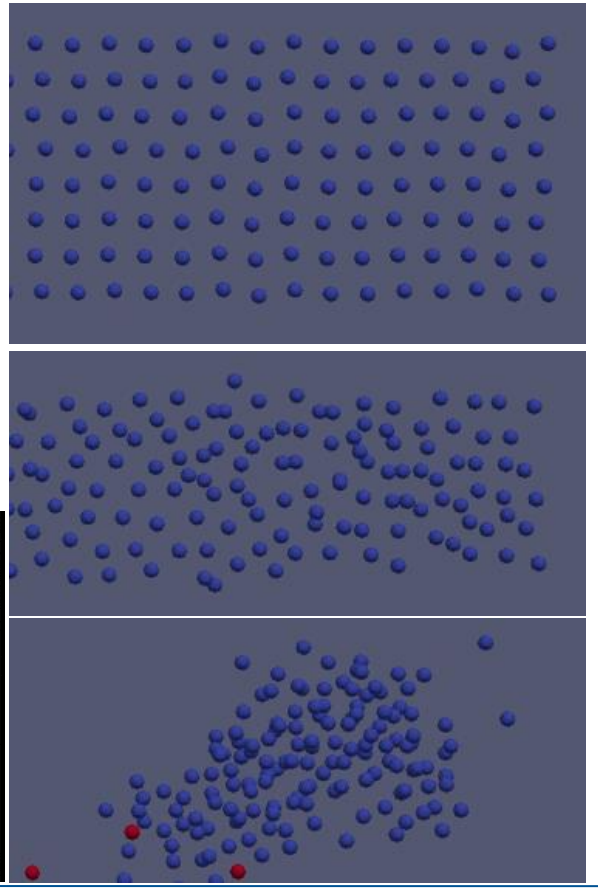
- The cuboids deform and seem to collapse a little even before collision
- Untouched portions of blue cuboid still deformed

-> **test with second simulation:** cube without initial velocity should become sphere-shaped

Similar processes:

- Forming of water drops
- Forming of (round) planets due to gravity





Simulation 2

Observations:

1. Order
2. Particles clump together
3. Particles that get too close drift apart again

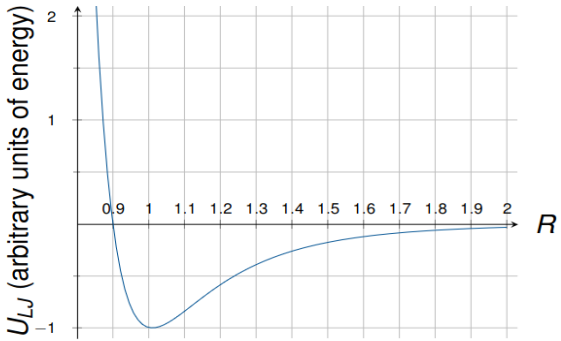
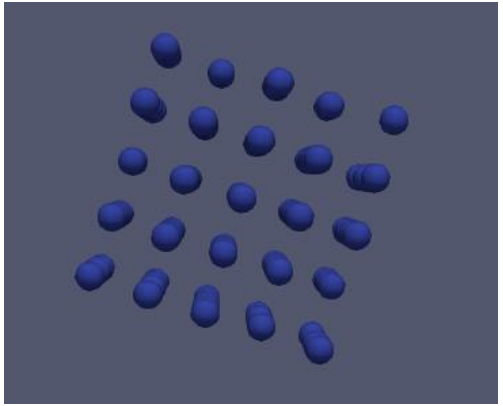
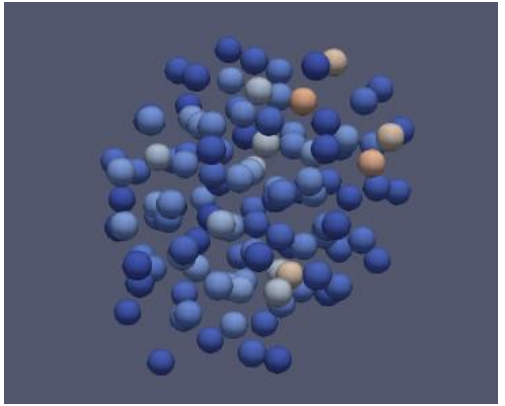
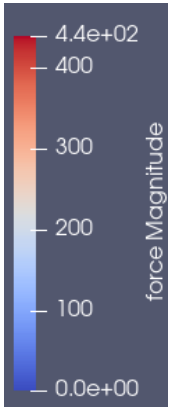


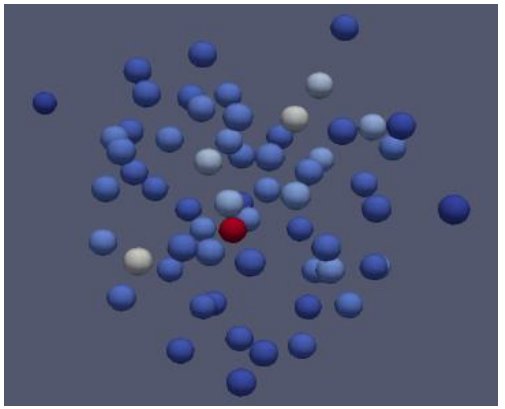
Abbildung: LJ-Potential for $\varepsilon = 1$ and $\sigma = 0.9$

-> asymmetry of Lennard-Jones-Potential









Summary of cool things

- We created a few tests
- We continued and marginally extended our GitHub workflow
- We simulated a bunch of particles
- We drew a pretty particle collision
- We drew an even prettier particle collision with a moving camera

References

- Unit testing bild: https://codefresh.io/learn/unit-testing/ 2
- Black box testing bild: https://www.imperva.com/learn/application-security/black-box-testing/
- Billiard balls colliding gif: https://community.wolfram.com/groups/-/m/t/418720
- Water droplet gif: https://popperfont.net/2012/08/20/superhydrophobic-carbon-nanotube-water-droplet-bouncing-gif-goodness/