

MolSim WS 23/24

Sheet 2

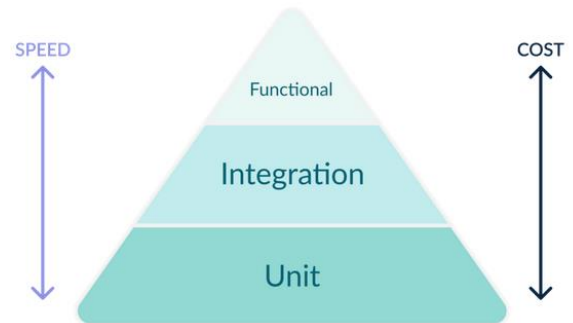
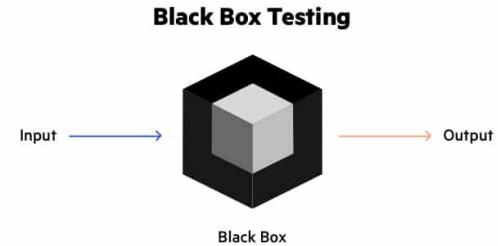
Collision of two bodies

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

The screenshot displays a GitHub Project Management interface for a project named 'MoSim-WS23-24'. The board is organized into three columns: 'Todo', 'In Progress', and 'Done'. The 'Todo' column contains three items, the 'In Progress' column is currently empty, and the 'Done' column contains seven completed items. Each item is represented by a card with a title and a brief description.

ManuellLerchner / Projects / MoSim-WS23-24

MoSim-WS23-24

View 1 + New View

Filter by keyword or by field

Todo 3
This item hasn't been started

- MoSim-WS23-24 #7
[Sheet 1] Refactor Codebase
- MoSim-WS23-24 #12
[Sheet 1] Create Presentation
- MoSim-WS23-24 #13
Default Timestep and Video

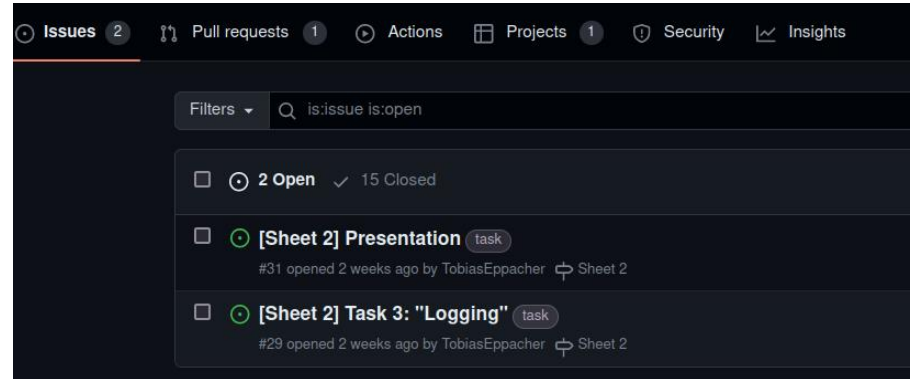
In Progress 0
This is actively being worked on

Done 7
This has been completed

- MoSim-WS23-24 #3
Implement Movement Calculations Sheet 1
- MoSim-WS23-24 #6
Implemented the 3 formulas and added setters to particle attributes
- MoSim-WS23-24 #1
add basic github convenience actions
- MoSim-WS23-24 #8
Pass arguments via comand line
- MoSim-WS23-24 #9
A bit of refactoring and command line input with boost_program_options
- MoSim-WS23-24 #10
Show help message when executed with no arguments;
- MoSim-WS23-24 #11
fix bug in formula

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

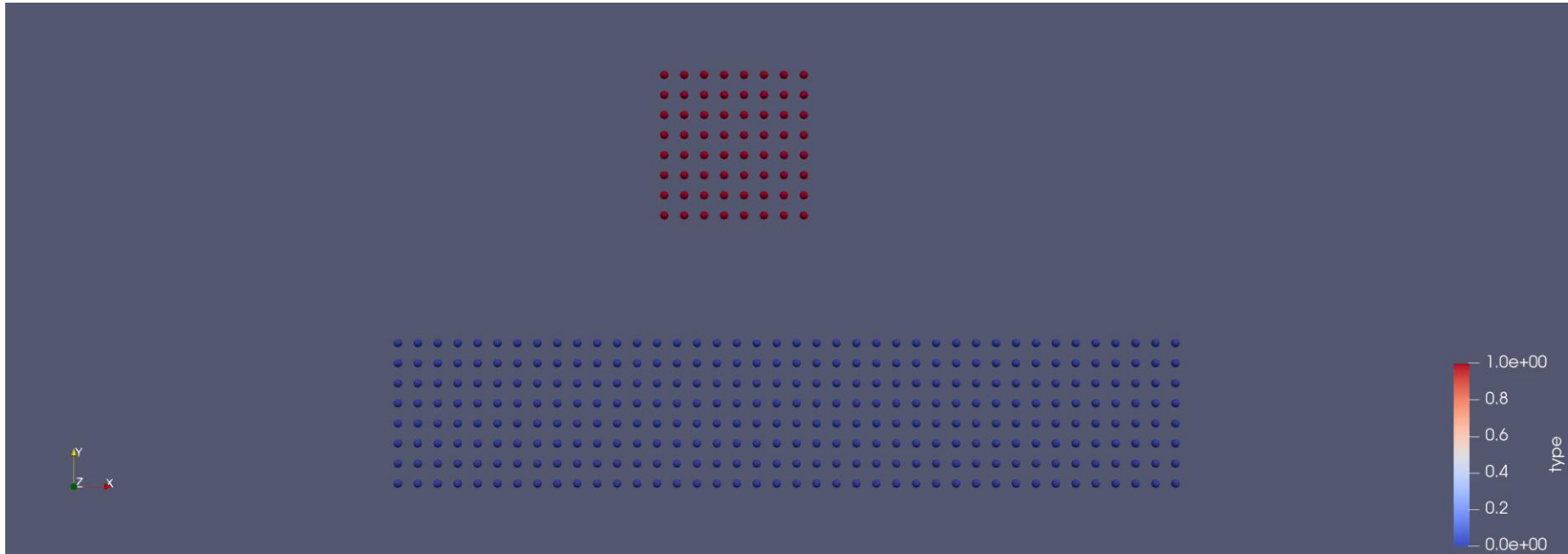
Prettier and distinguishable output for different information

User selectable log-levels

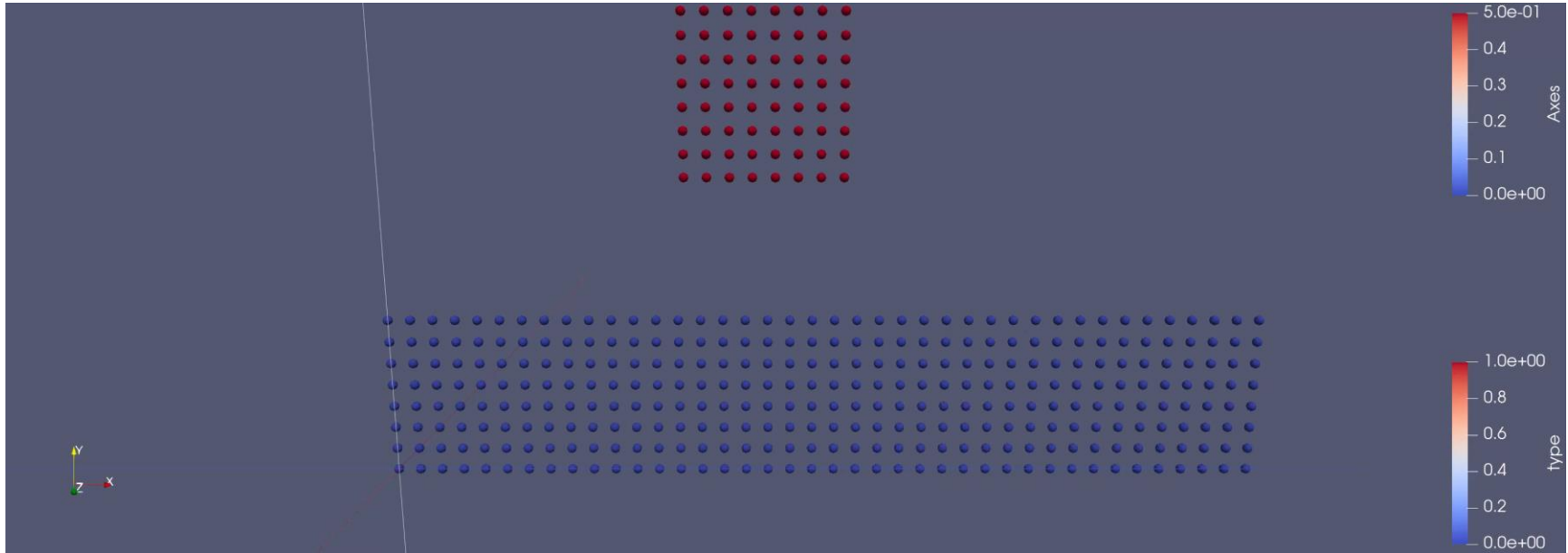
```
[18:49:54] [info] Simulation arguments:
[18:49:54] [info] Input file path: ../../input/body_collision.cub
[18:49:54] [info] Output directory path: ./output/body_collision/
[18:49:54] [info] End time: 5
[18:49:54] [info] Frames per second: 24
[18:49:54] [info] Video length: 30
[18:49:54] [info] Log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

Simulation 1



Simulation 1



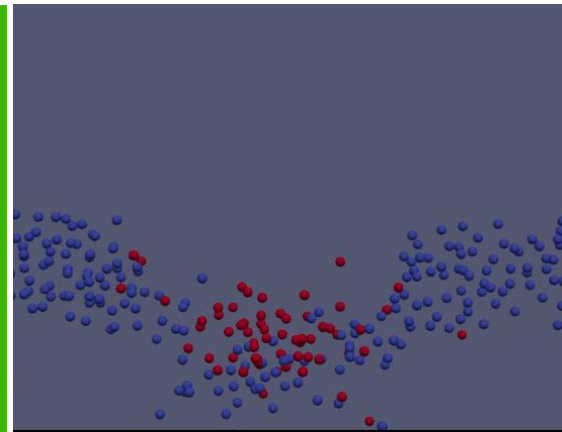
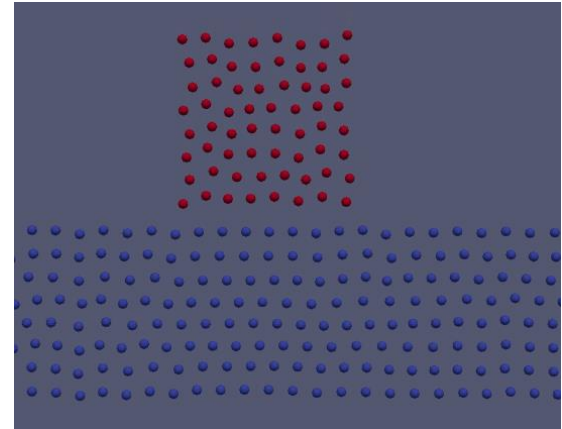
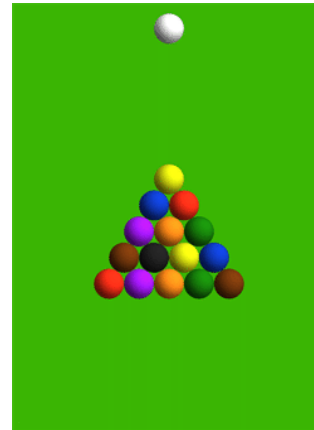
Simulation 1

Observation 1:

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

Similar processes:

- Billiard ball colliding



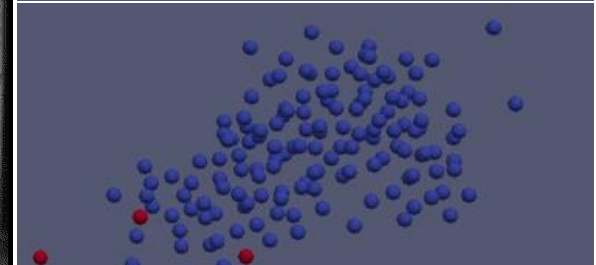
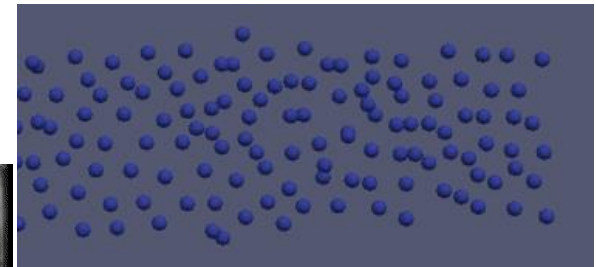
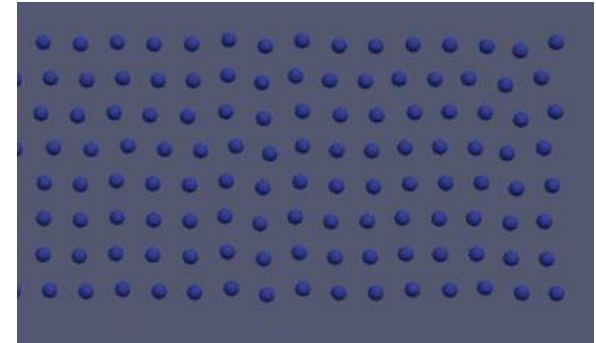
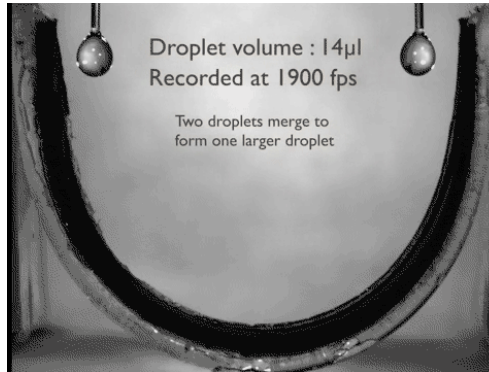
Simulation 1 + 2

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

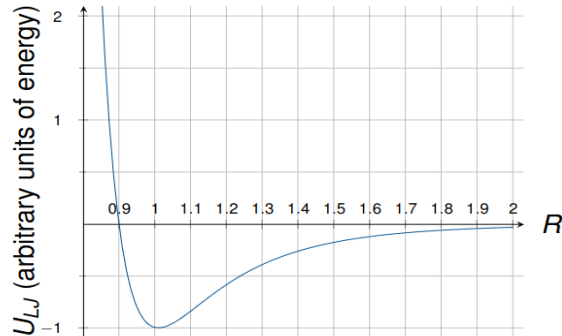
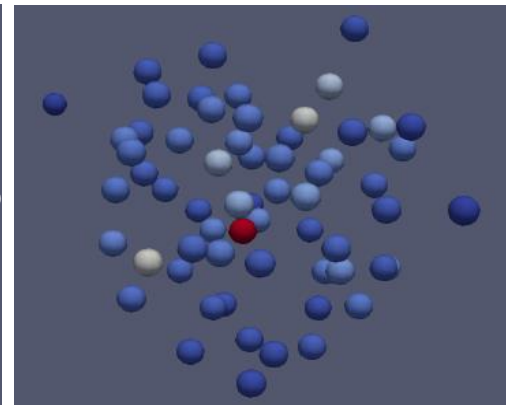
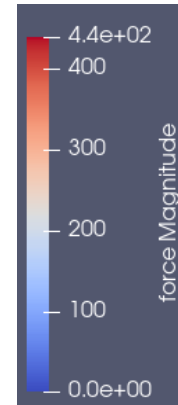
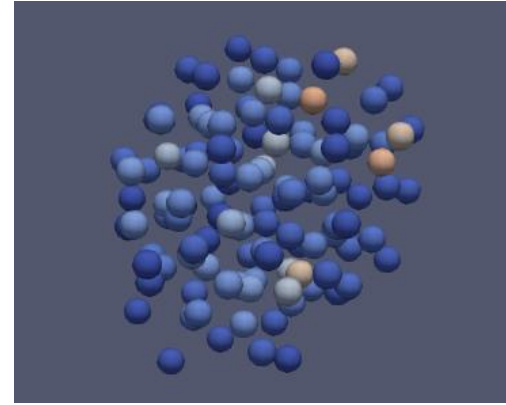
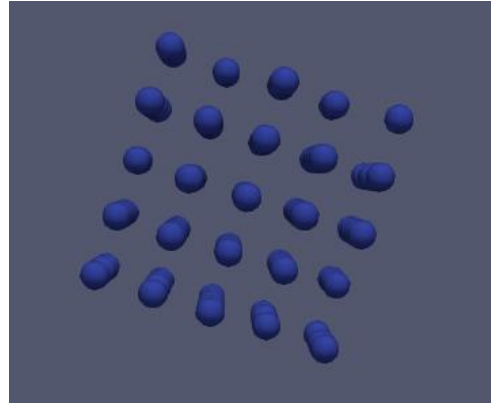


Abbildung: LJ-Potential for $\epsilon = 1$ and $\sigma = 0.9$

-> **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/>