

MolSim WS 23/24

Sheet 4

Thermostats, Rayleigh-Taylor instability, “Falling Drop” and Performance Measurement

Group C [Manuel, Tobias, Daniel]

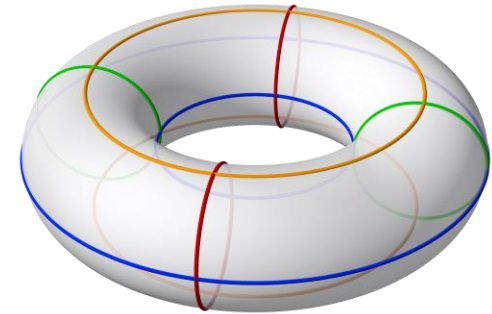
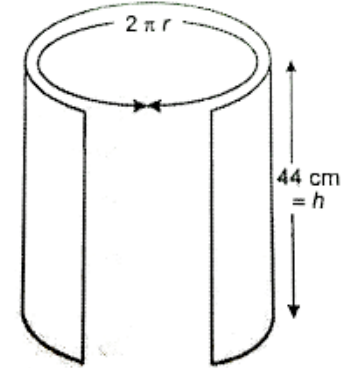
22.12.2023

Thermostats

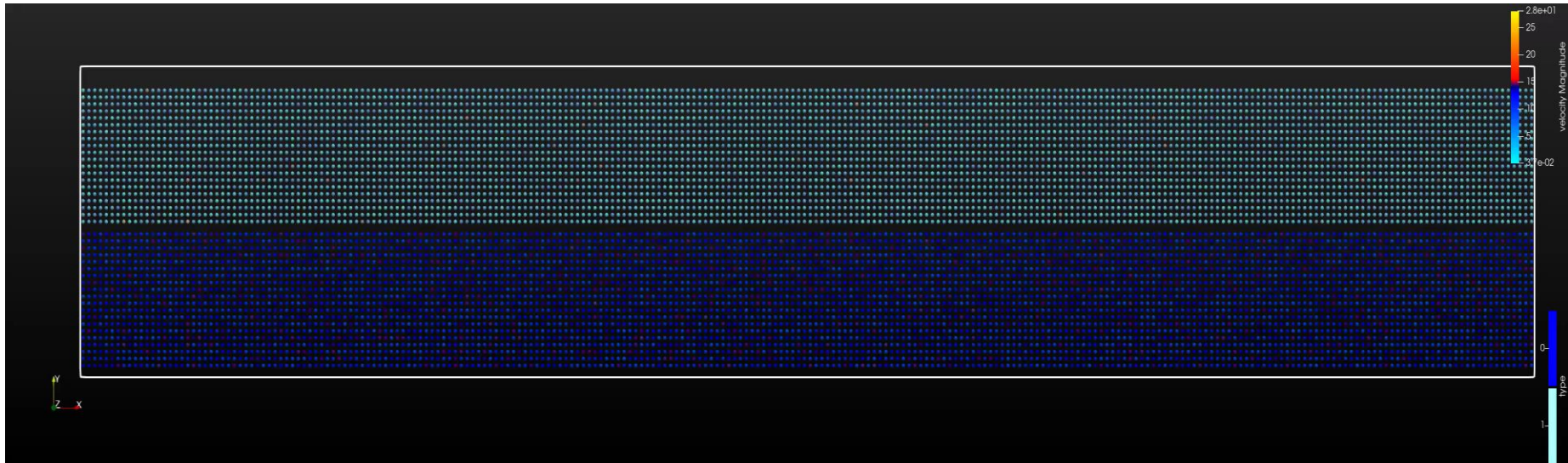
- **Global scaling**
 - Simple loop using $\beta := \sqrt{\frac{T_{new}}{T_{current}}}$
- **Concept of Interceptors**
 - We group all functions performed once all N iterations under **interceptors**
 - e.g. Thermostats, FileWriter ...

Periodic boundaries

- **First idea:**
 - Fold the rectangle shaped domain to cylinder
⇒ problems with distance calculation
- **Implementation:**
 - Teleport particles manually to the other side



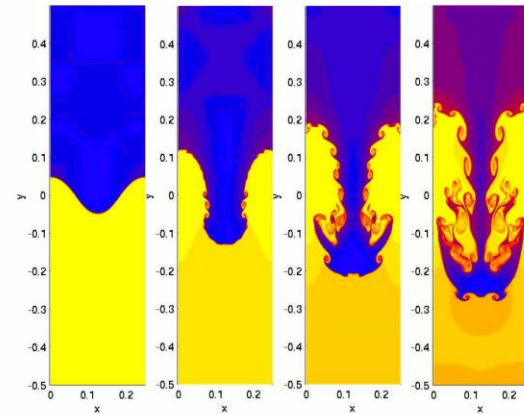
Rayleigh-Taylor instability



<https://manuellerchner.github.io/MoISim-WS23-24/submissions/>

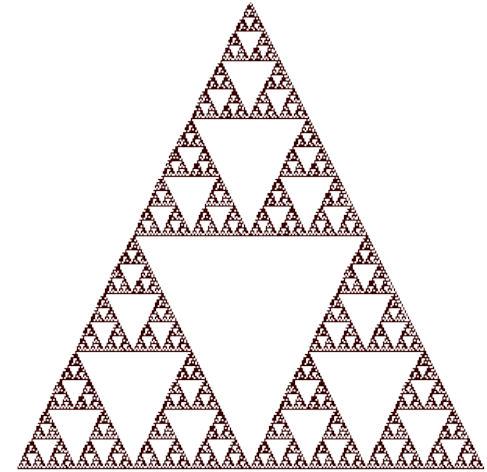
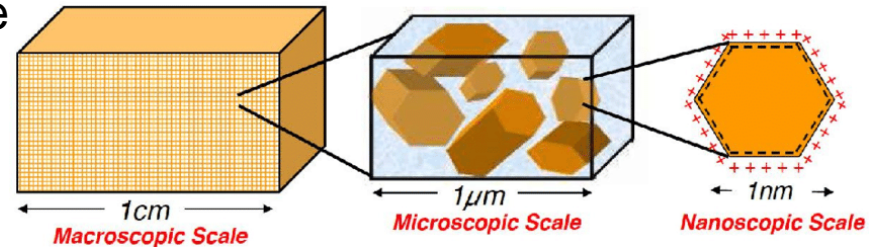
Rayleigh-Taylor instability

- **Observations:**
 - Lower fluid shooting up
 - Effect emerging through broken symmetry in upper fluid
- **Analogy:**
 - Mushroom cloud of an atom bomb

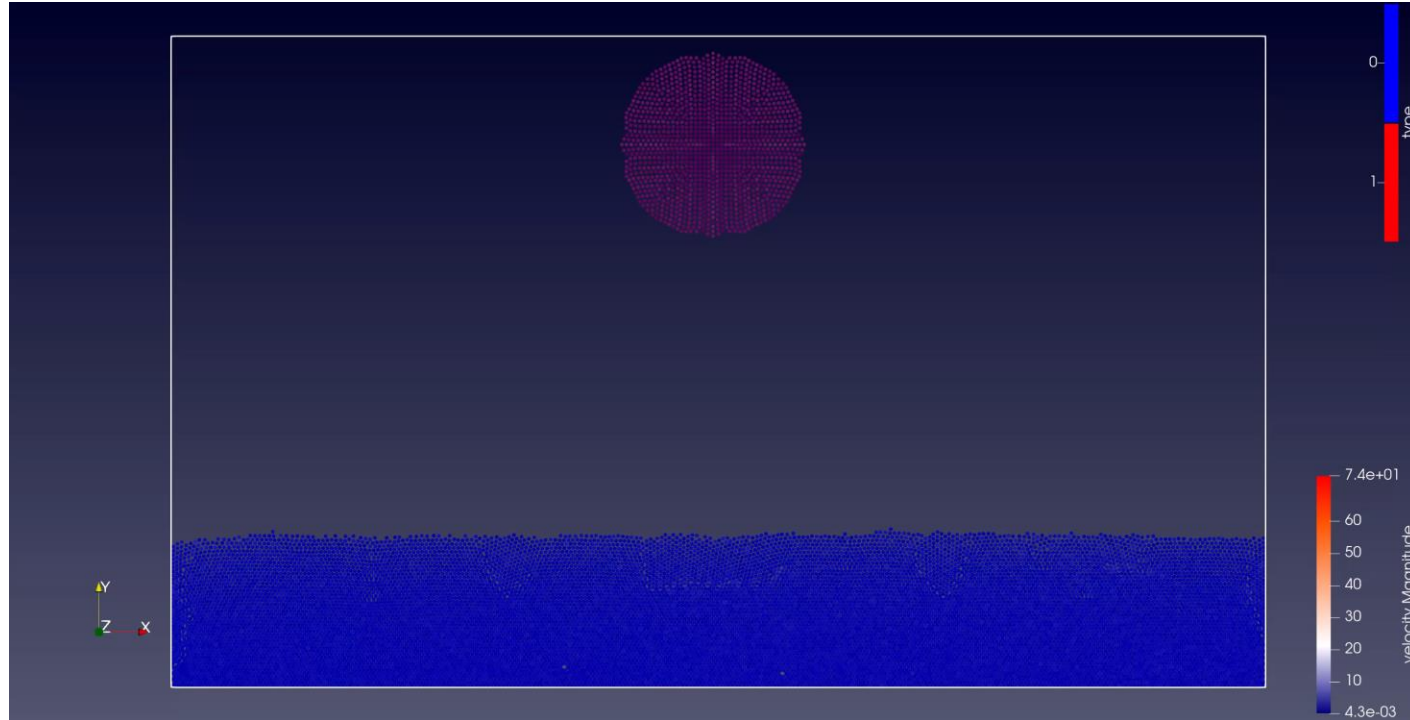


Simulation of a falling drop

- **Equilibration:**
 - We implemented the equilibration recursively
 - User is able to create subsimulations to build a large system from small parts
 - This mechanism lets the user create multiple scales intuitively

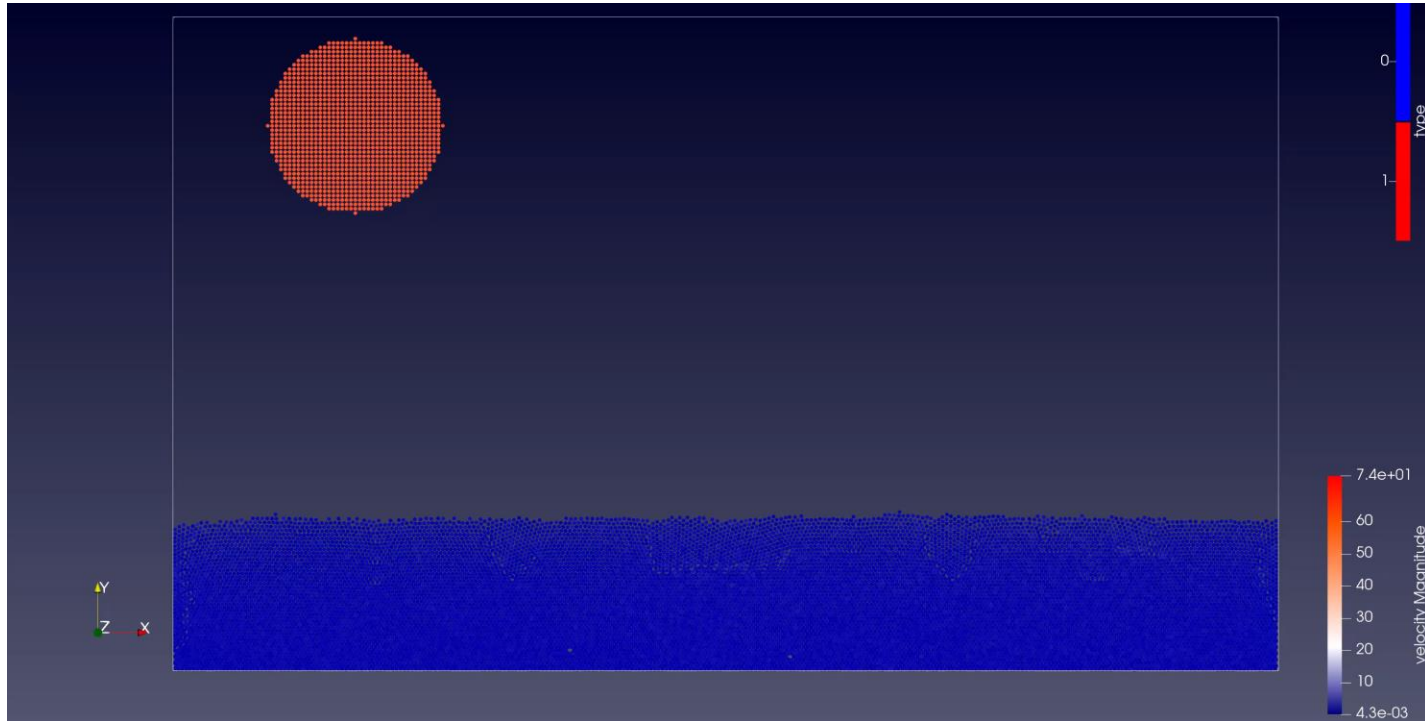


Simulation of a falling drop



<https://manuellerchner.github.io/MolSim-WS23-24/submissions/>

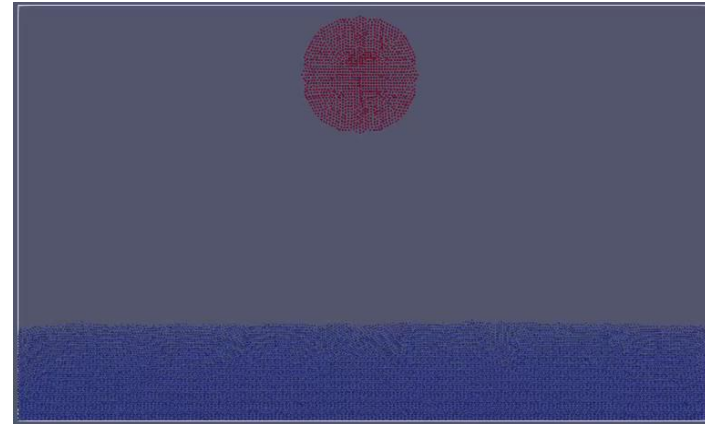
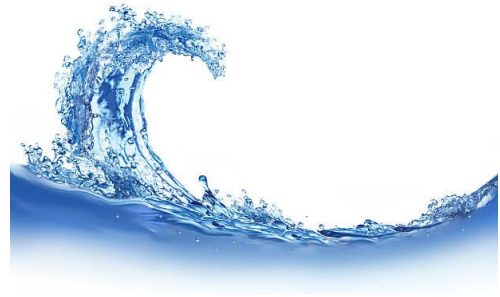
Simulation of a thrown drop



<https://manuellerchner.github.io/MolSim-WS23-24/submissions/>

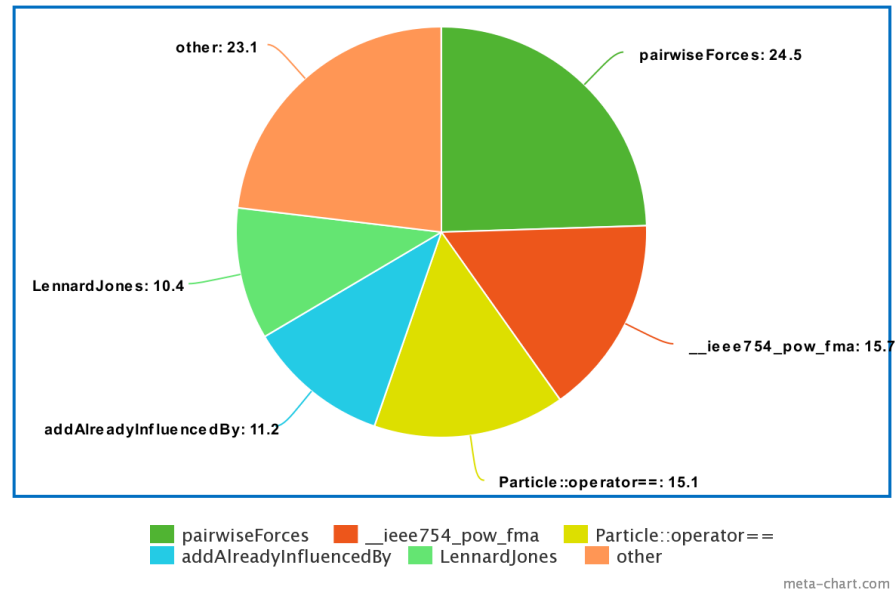
Simulation of a falling drop

- **Observations:**
 - The simulation really resembles a real fluid
 - Visible, big waves distributing into many smaller waves like in reality
 - In the thrown version even a surfing-like wave
- **Remark:**
 - Temperature is very important in this simulation
 - Creating different states of matter



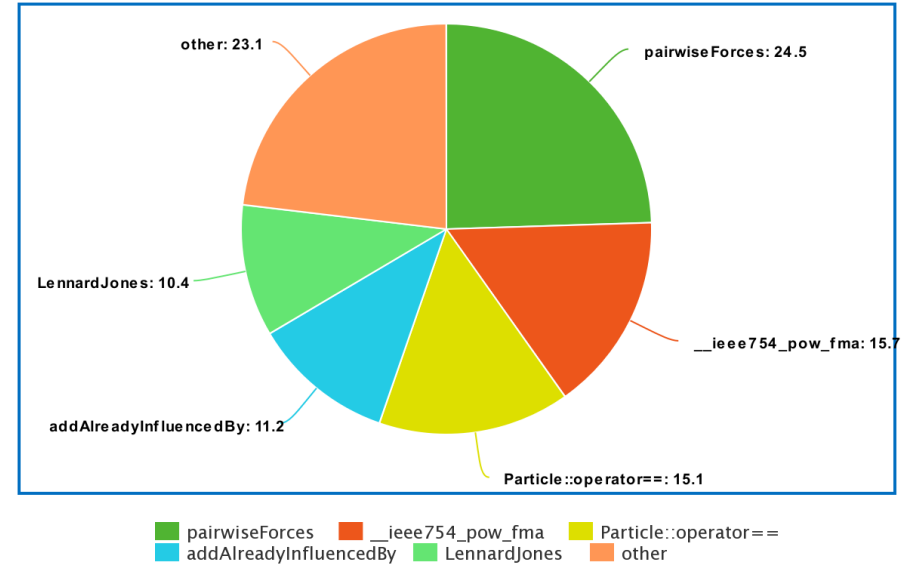
Performance measurement

- **Performance + Profile:**
 - The cluster took ____ s with ____ MUP/s
- **Idea:**
 - Calculate Lorentz-Berthelot mixing rule outside of the loop



Performance tuning

- **Performance + Profile after idea:**
 - The cluster took ____ s with ____ MUP/s after the implementation



meta-chart.com

Summary of cool things

- We failed making a cool torus domain
- We implemented thermostats to control temperature
- We simulated funky liquids
- We created a fancy water drop simulation
- We created a sad falling snowball simulation
- We drew a pretty profile plot

References

Torus picture: https://upload.wikimedia.org/wikipedia/commons/thumb/1/17/Tesseract_torus.png/1500px-Tesseract_torus.png

Cylinder picture: <https://www.doubtnut.com/qna/32538537>

Rayleigh-Taylor instability pic : https://en.wikipedia.org/wiki/Rayleigh%E2%80%93Taylor_instability

Macro vs microscopic: https://www.researchgate.net/figure/Macroscopic-microscopic-and-nanoscopic-portraits-in-kaolinite_fig1_226836400/download?tp=eyJjb250ZXh0Ijp7ImZpcnN0UGFnZSI6Il9kaXJlY3QiLCJwYWdlIjoieXZlcmVjZCJ9fQ

Recursion pic: <https://www.usna.edu/Users/cs/nchamber/courses/si204/s18/lec/l24/lec.html>