MolSim WS 23/24

Sheet 4

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

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Thermostats

- **Global scaling**
  - Simple loop using $\beta := \sqrt{\frac{T_{new}}{T_{current}}}$
- **Concept of Interceptors**
  - We group all functions performed once all

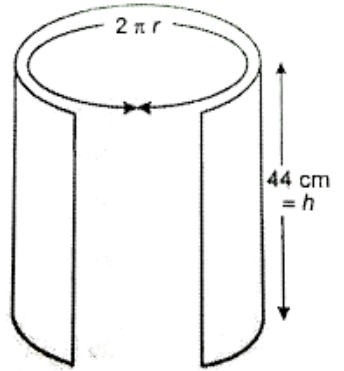
  N iterations under **interceptors**
  - e.g. Thermostats, FileWriter ...

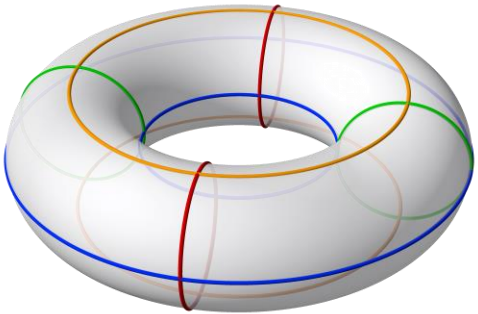
Periodic boundaries

- **First idea:**
  - Fold the rectangle shaped domain to cylinder

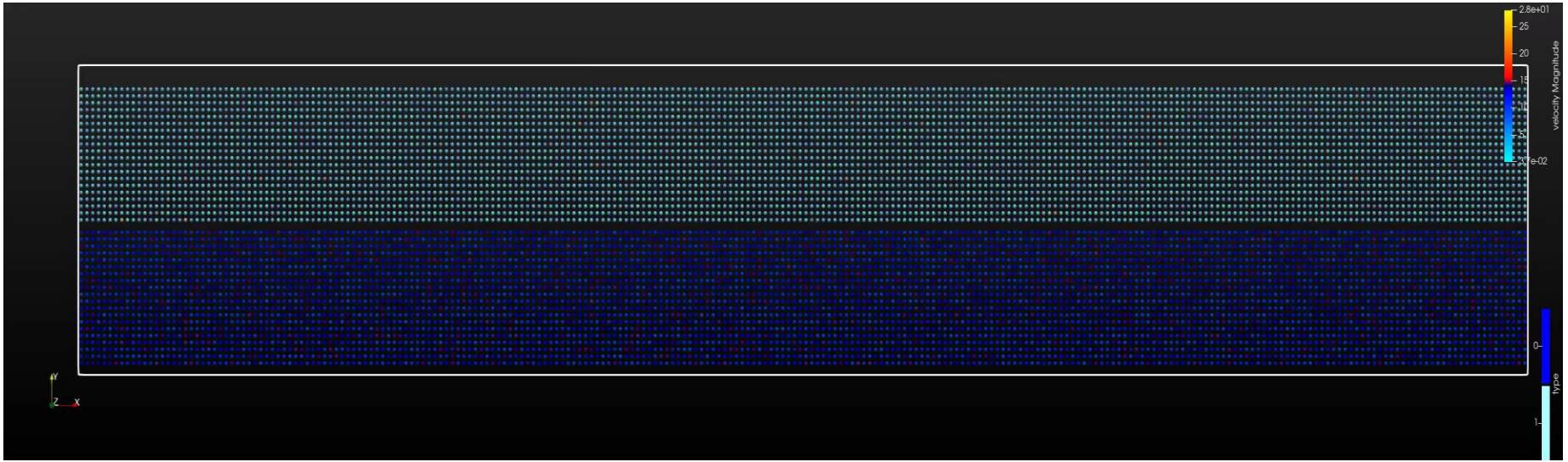
  ⇒ problems with distance calculation

- **Implementation:**
  - Teleport particles manually to the other side





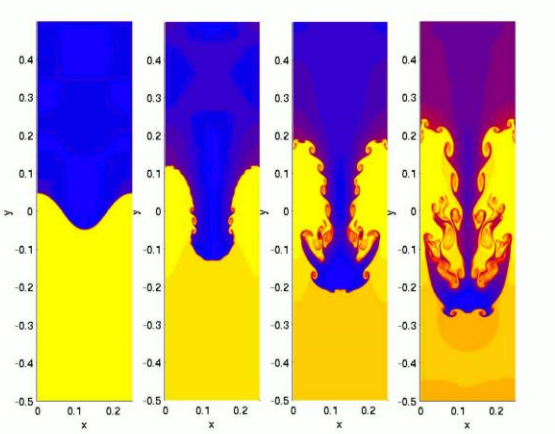
Rayleigh-Taylor instability



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

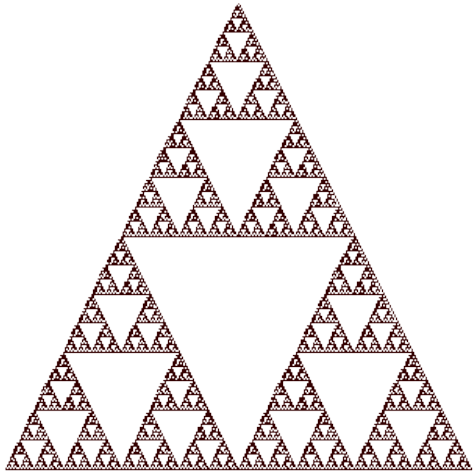
Rayleigh-Taylor instability

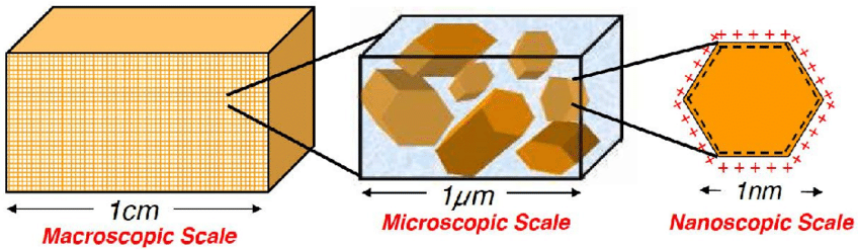
- **Observations**:
  - Lower fluid shooting up
  - Effect emerging through broken symmetry in upper fluid
- **Analogy**:
  - Mushroom cloud of an atom bomb



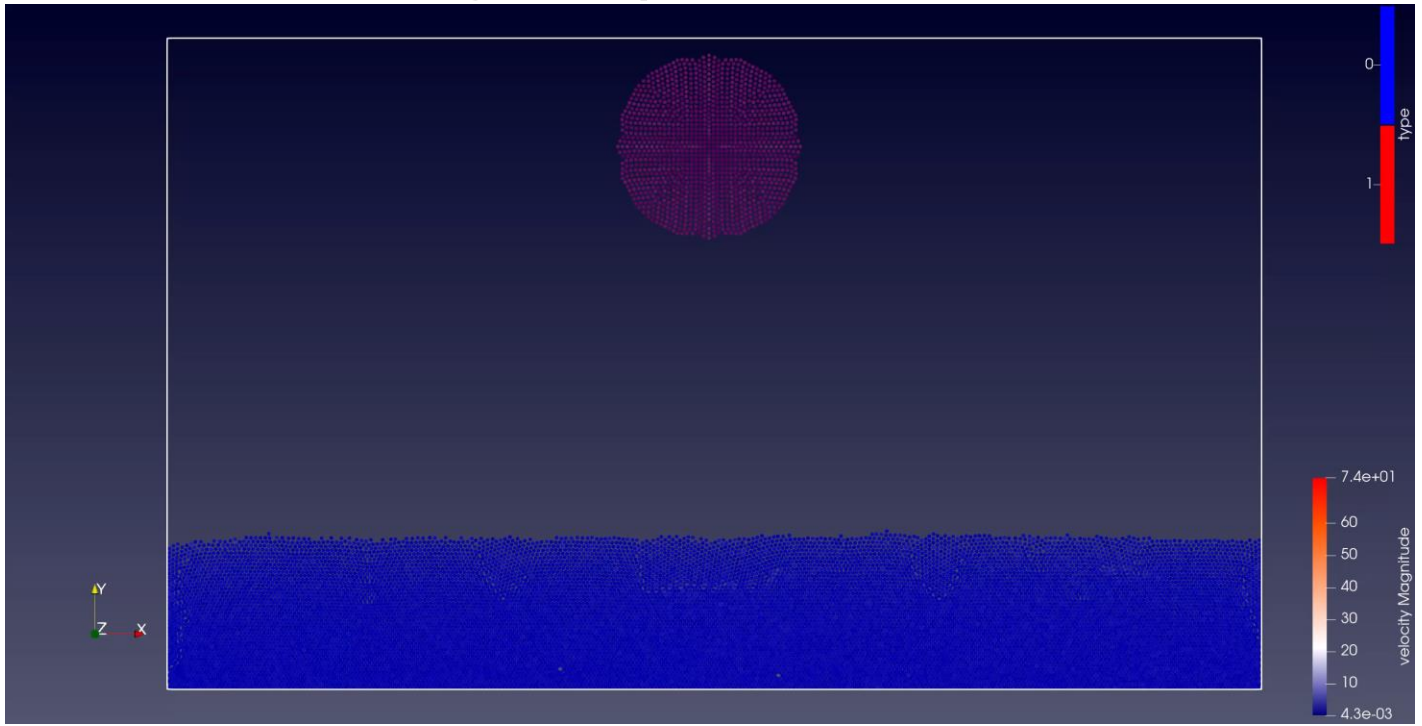
Simulation of a falling drop

- **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



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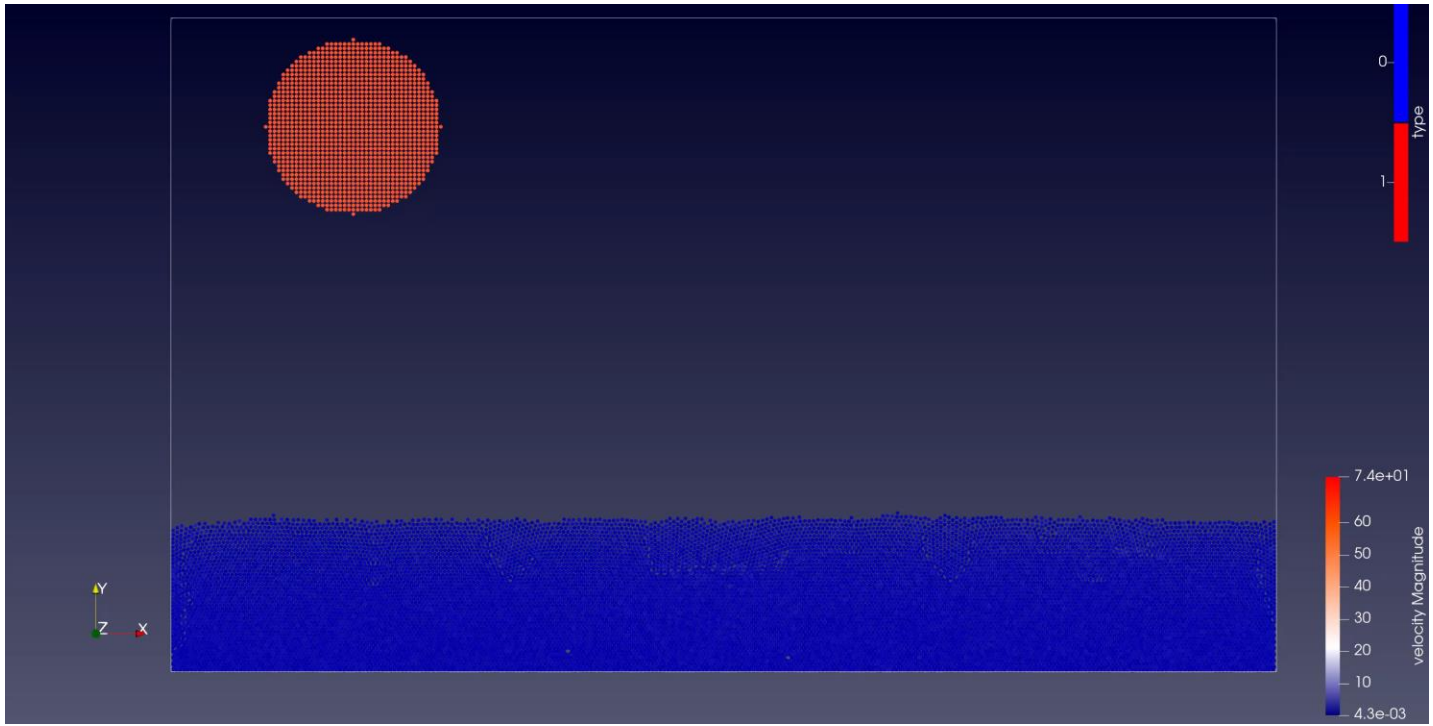
Simulation of a thrown drop



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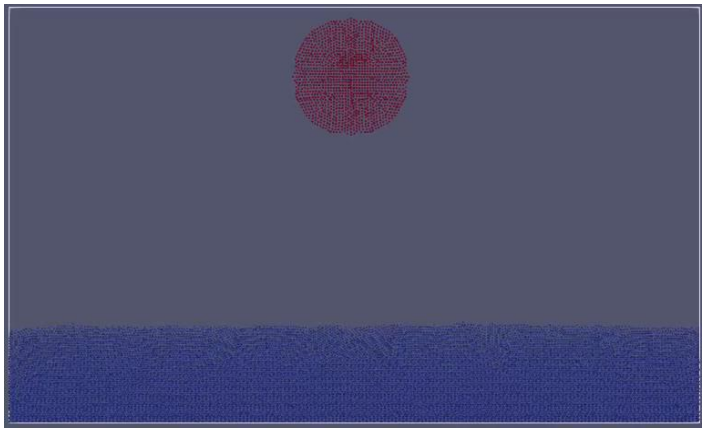
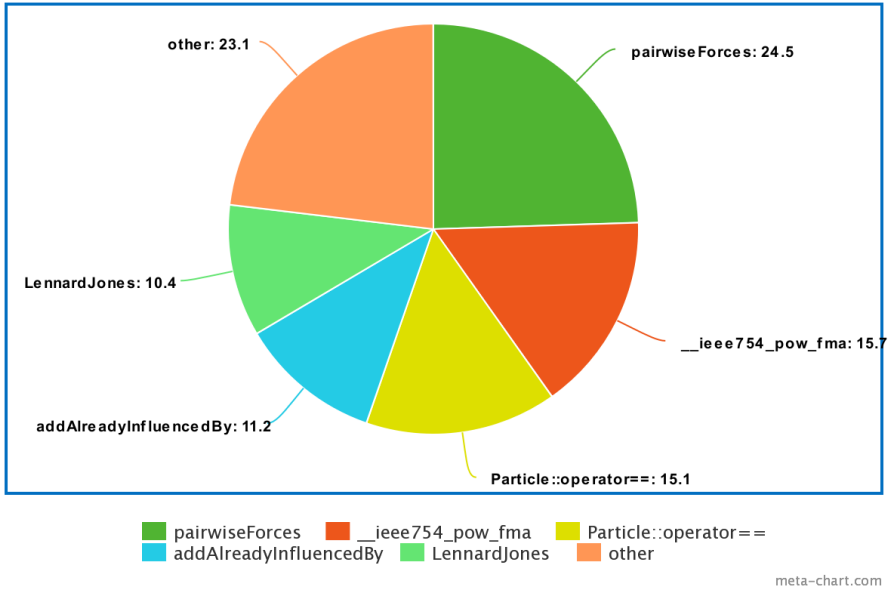
Simulation of a falling drop

- **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



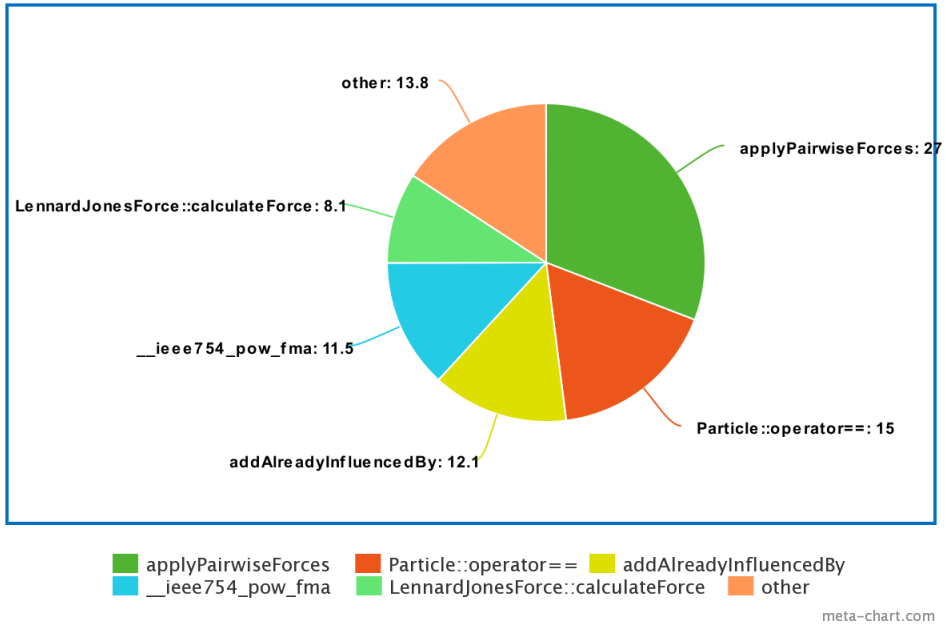
Performance measurement

- **Performance + Profile:**
  - The cluster took 42s 476ms with 282960 MUP/s
- **Idea**:
  - Calculate Lorentz-Berthelot mixing rule outside of the loop



Performance tuning

- **Performance + Profile after optimization:**
  - The cluster took 42.485s with 233355 MUP/s after the implementation
  - Did not work :/
  - Mapping logic creates overhead



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=eyJjb250ZXh0Ijp7ImZpcnN0UGFnZSI6Il9kaXJlY3QiLCJwYWdlIjoiX2RpcmVjdCJ9fQ
Recursion pic: https://www.usna.edu/Users/cs/nchamber/courses/si204/s18/lec/l24/lec.html
Wave pic: https://media.istockphoto.com/id/120917341/de/foto/cool-water-wave.jpg?s=612x612&w=0&k=20&c=Ky3AZFWCoLQhKgW6j_TxG_HF6Ci4Cifj1_tUPAq5ypE=