Bachelor-Praktikum - Scientific Computing
Molecular Dynamics
(PSE)

Worksheet 4 – Molecule Simulation

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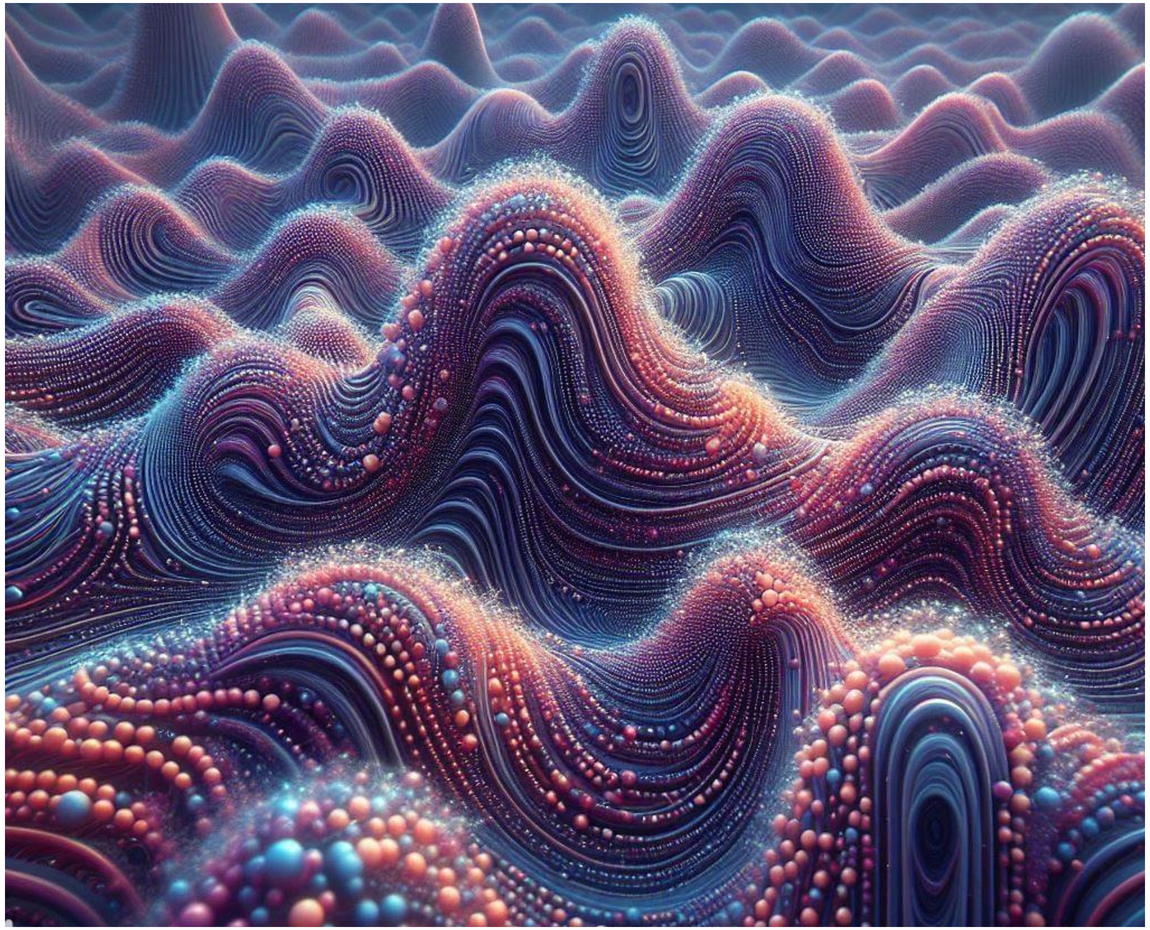
Periodic Boundaries: Particle Continuity in Simulations

- For each boundary, check if periodic boundary conditions are applied and if the particle has crossed the boundary

- If a lower boundary is crossed, update the particle's position by adding the size of the respective axis to the current axis position, ensuring that the particle reappears on the upper boundary.

- If an upper boundary is crossed, update the particle's position by subtracting the size of the respective axis from the current axis position, ensuring that the particle reappears on the lower boundary.

- Final result: All particles smoothly wrap around the simulation space from periodic boundaries, maintaining a continuous and periodic simulation environment.



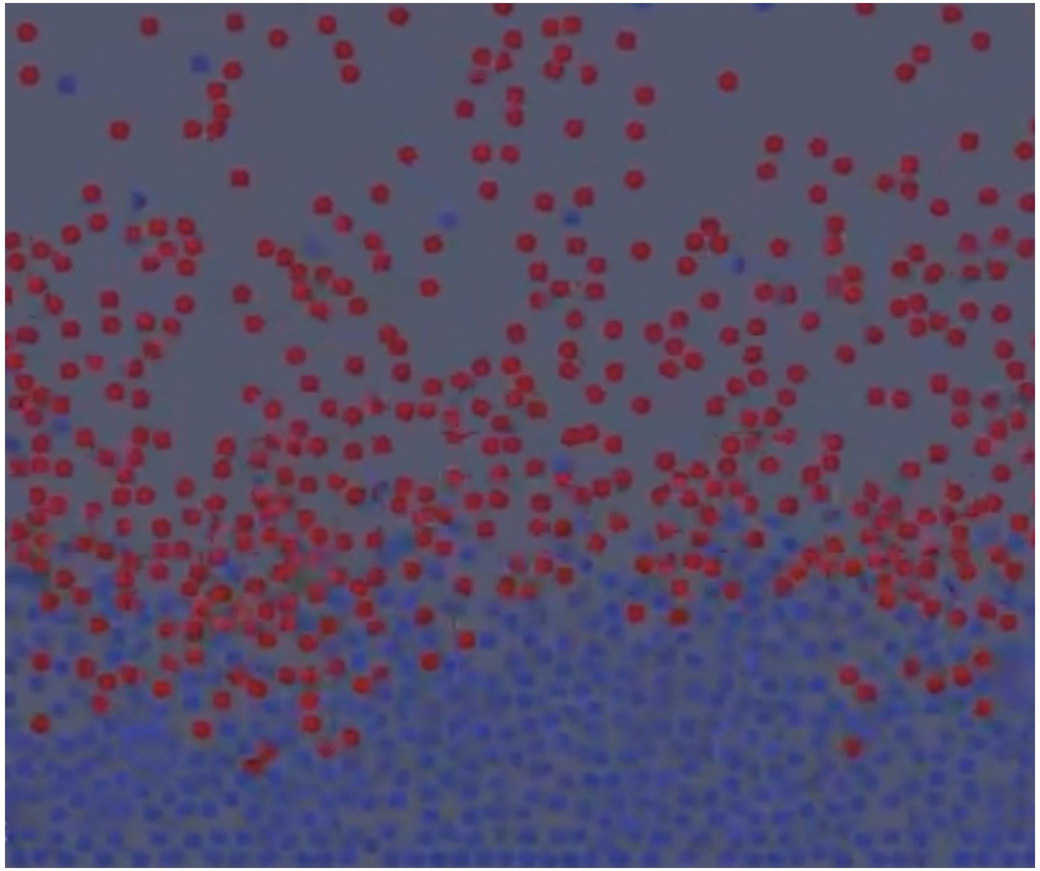
Periodic Boundaries: From Boundary to Opposite Halo Layer

Brief Explanation of the Algorithm:

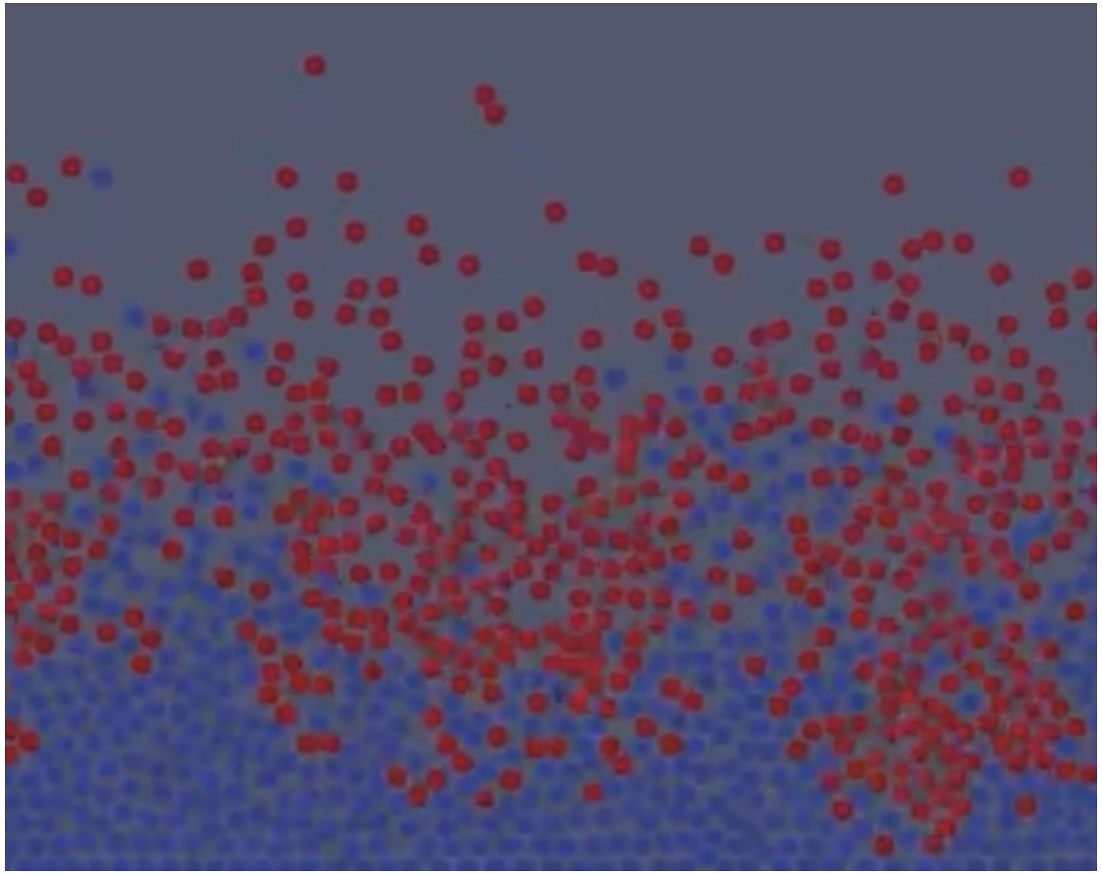
- Converts boundary cell indices to 3D coordinates, sets one of the positions to 0 or axis size – 1, depending on upper/lower boundary
- Then converts the updated 3D index back to a 1D index representing the halo cell
- Then it iterates through all particles in the boundary cell (for which the index was given as parameter) and creates new particles with the updated position and the same velocity, mass, and other properties
- Finally adds these new particles to the halo cell for which the index was calculated earlier

Important: The algorithm checks if the condition for the boundary cell is periodic and if so, then copies it as halo cell to the other side of the boundary

Why is Thermostat Important for the Simulation?



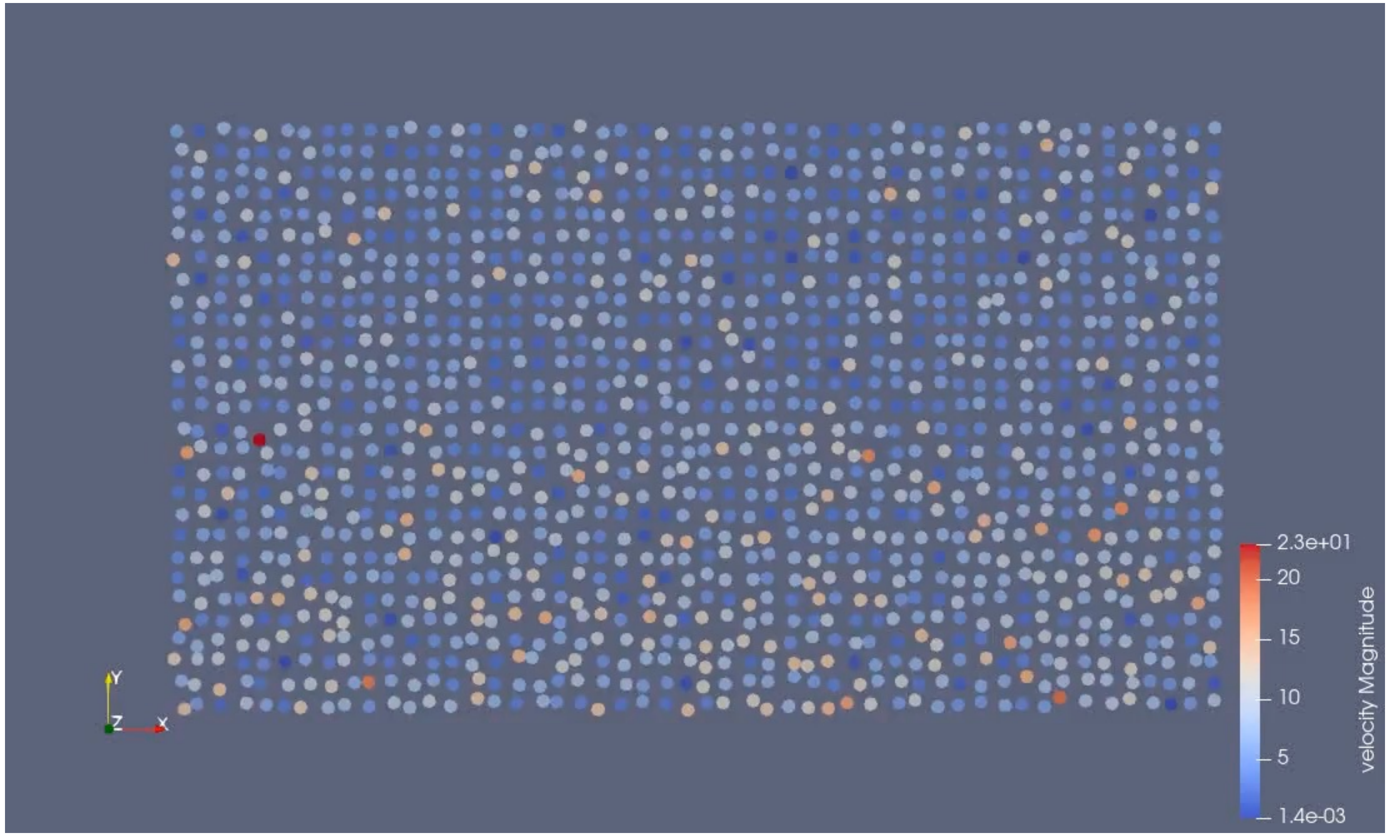
Without Thermostat



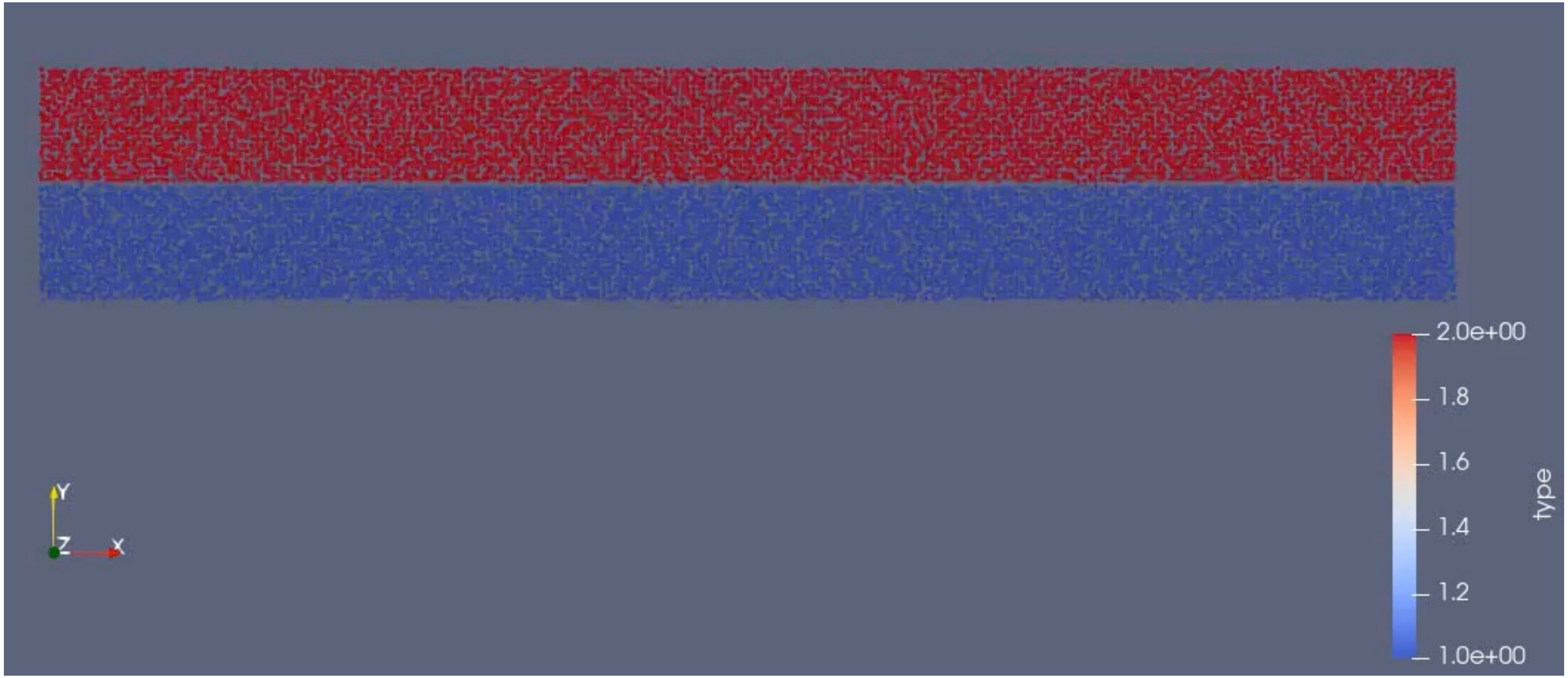
With Thermostat

How Did We Implement the Thermostat?

- Allows gradual and direct scaling of particle velocities based on temperature differences.
- Optional Brownian Motion and Safeguards: Against issues like division by zero for 'invalid' temperatures.
- Future Plans: Google Mocks for Testing and handling sub-zero temperatures



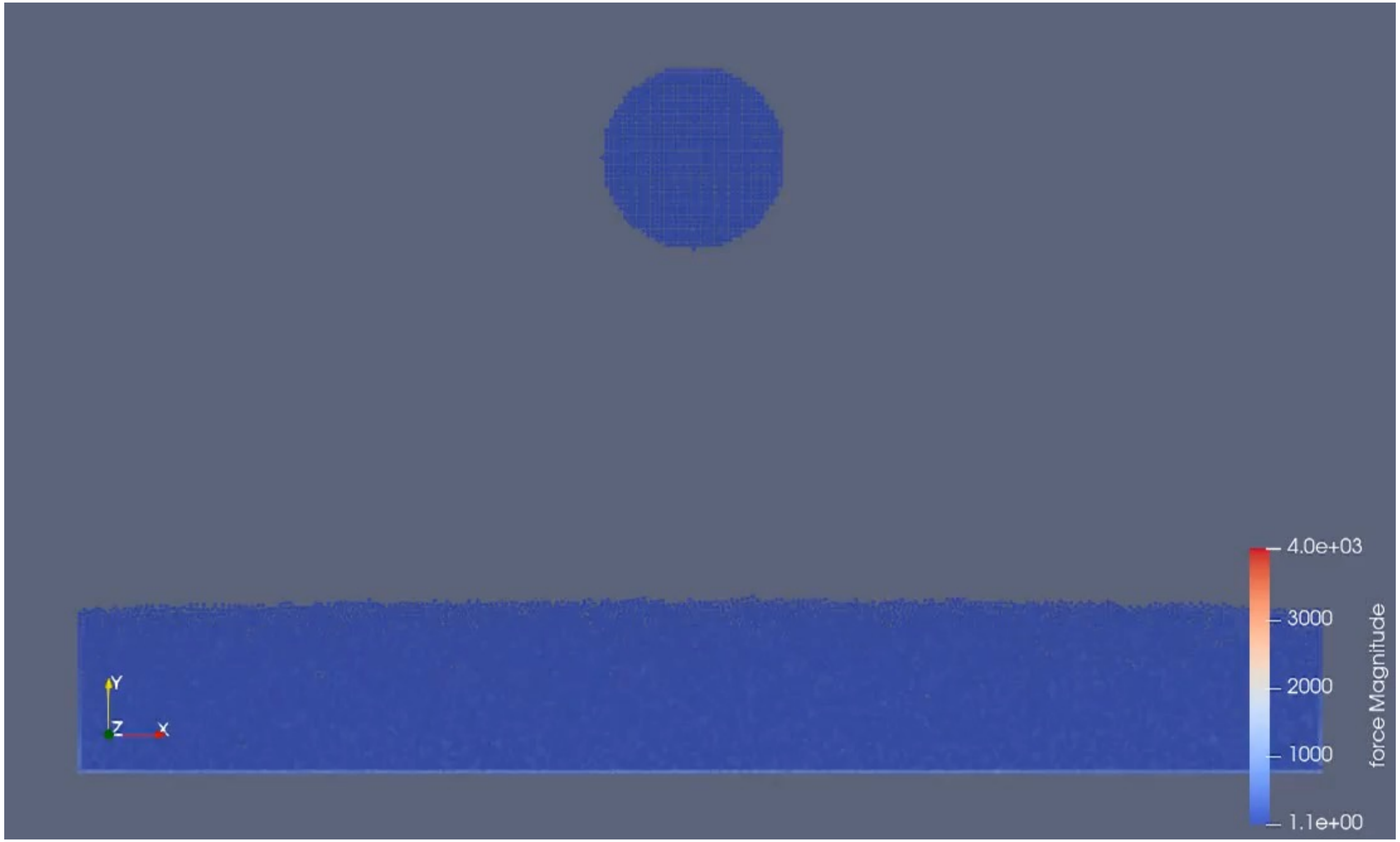
Rayleigh-Taylor-Instability



- Mixing rules
- Gravity…

The Falling Drop

- Checkpointing



Problems Encountered

- We mistakenly applied the gravity force on the particles for each iteration in the ‘ApplyToAllPairs’ instead of ‘ApplyToAll’
→ On the particles with many other neighboring particles, the gravity was applied too heavily, many particles just collapsed to the ground because of a gravity force comparable to of a giant planet rather than Earth’s

- We mixed up the periodic boundary condition for halo cell update, e.g. we copied the particles from the lower boundary cell to the upper halo cell, if the upper boundary is periodic but for that we should have checked, if the lower boundary is periodic

Problems Encountered

- We thought we had a problem with the reflection algorithm, so we changed it multiple times, trying to cover even more edge cases

→ Turns out the problem was that we haven’t been using the thermostat, so particles reach absurd velocities and thus also positions such as (x: 10000, y, z), therefore they had to be reflected thousands of times, bottlenecking the simulation

References

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