

# Molecular Dynamics - Assignment 4

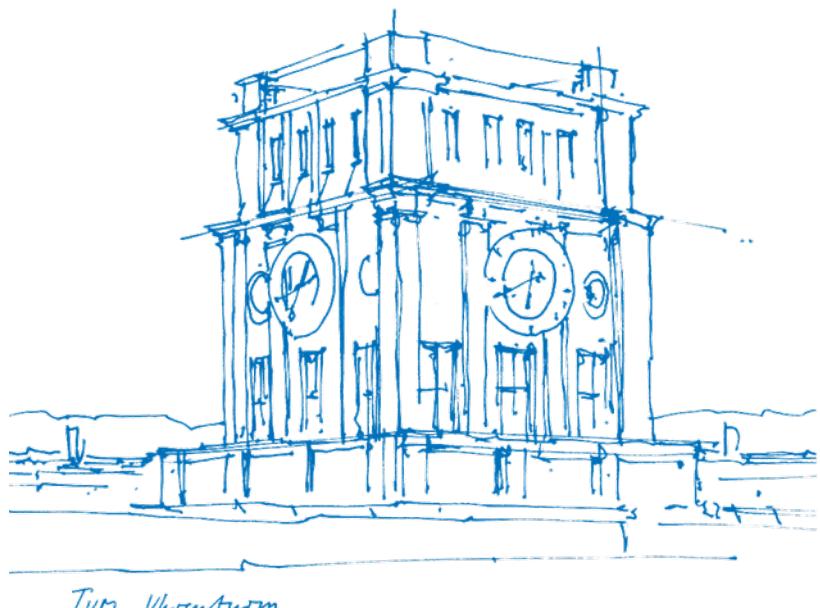
Alex Hocks Jan Hampe Johannes Riemenschneider

Technische Universität München

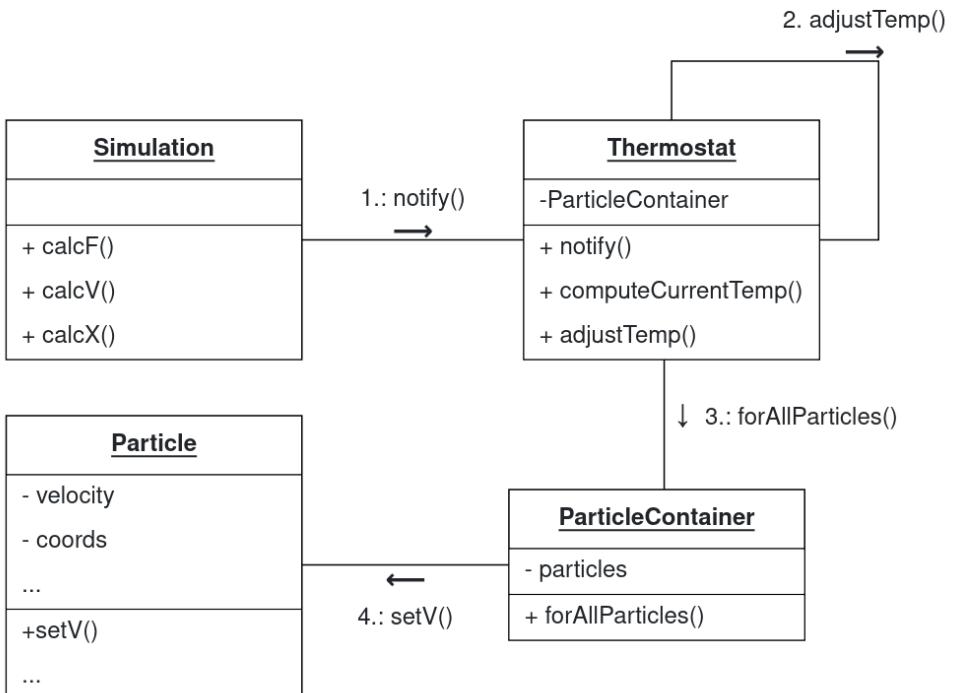
TUM CIT

Lehrstuhl für wissenschaftliches Rechnen

20. Dezember 2022



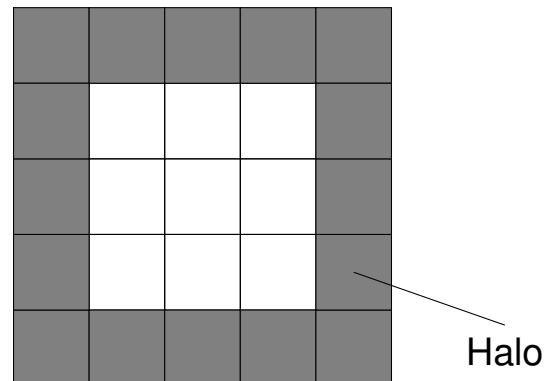
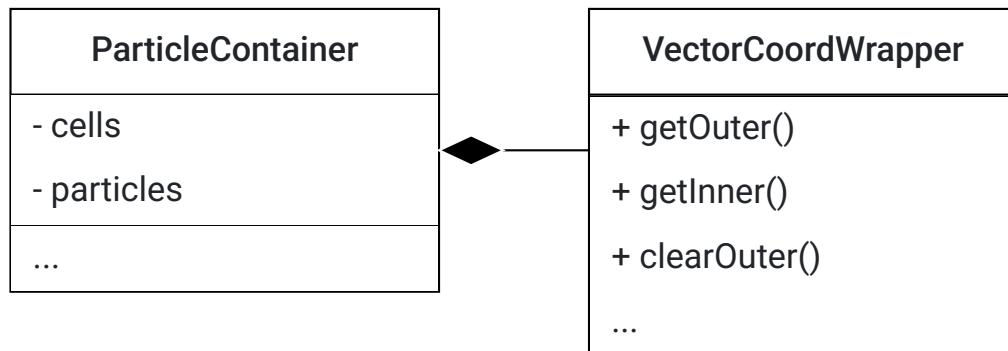
# Thermostat



# Adapting ParticleContainer for periodic bounds

Idea:

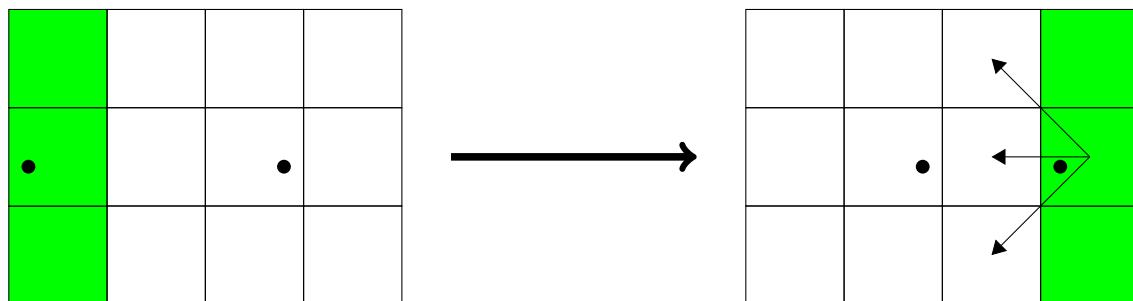
- Provide virtual cells around the actual domain for anyone who needs it
- Existence of additional cells is invisible with old interface



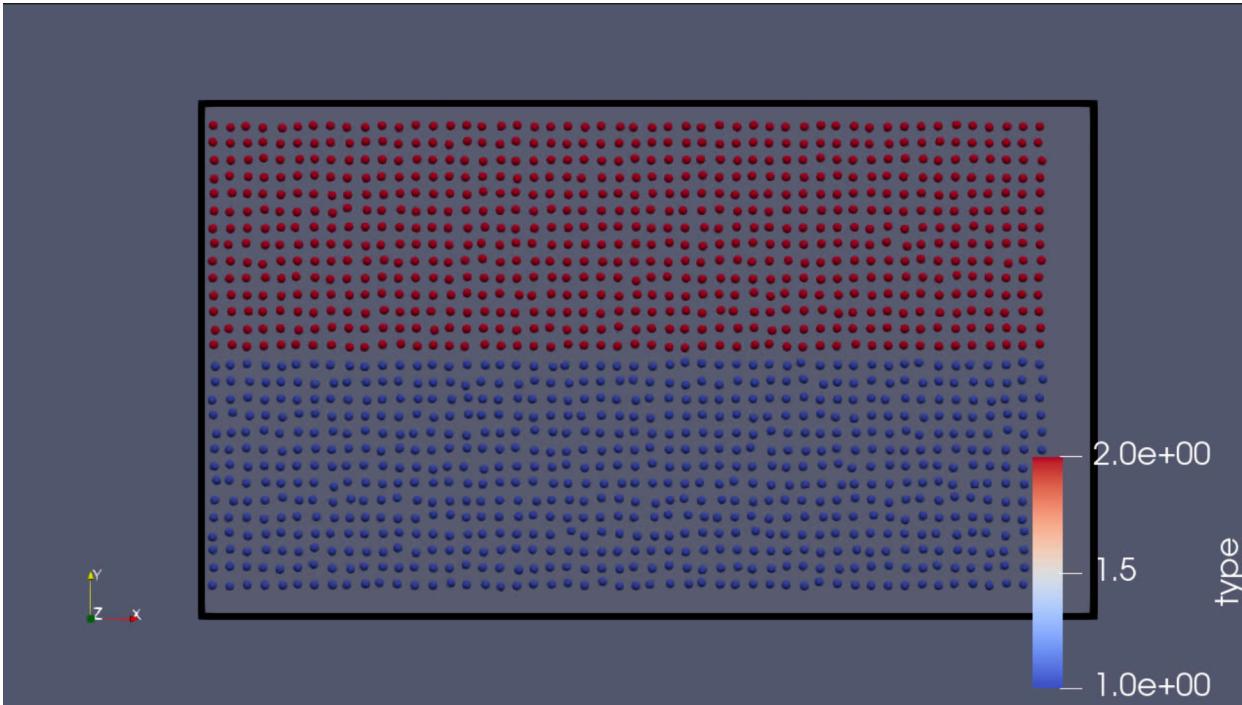
# Boundary conditions

Idea:

1. Temporarily move all particles next to Boundary of the other side
2. Let Neighbouring cells interact

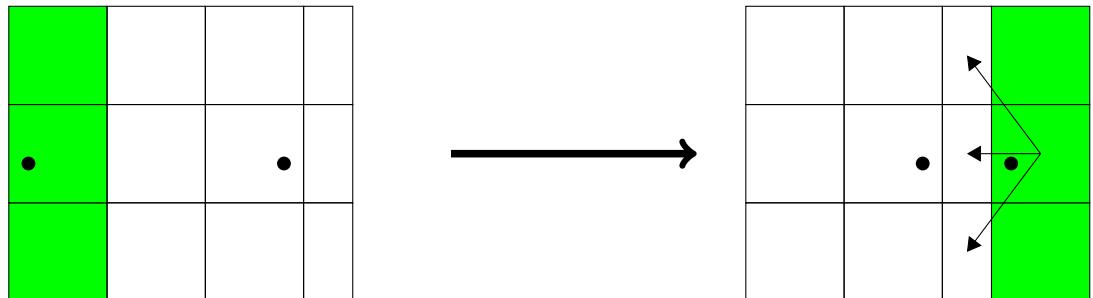


# The result



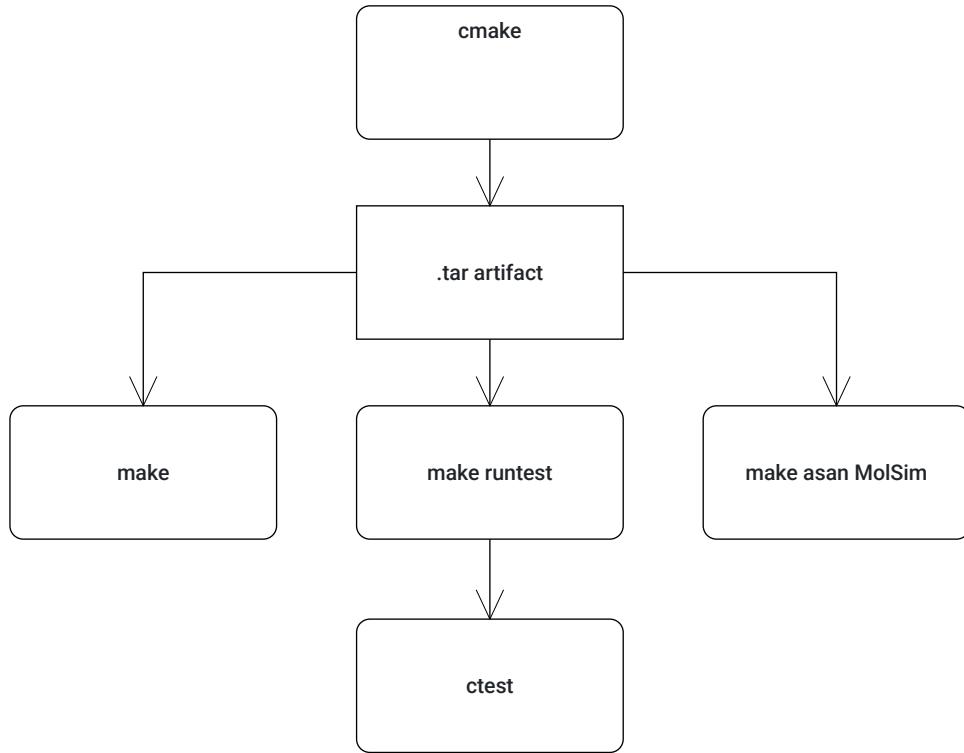
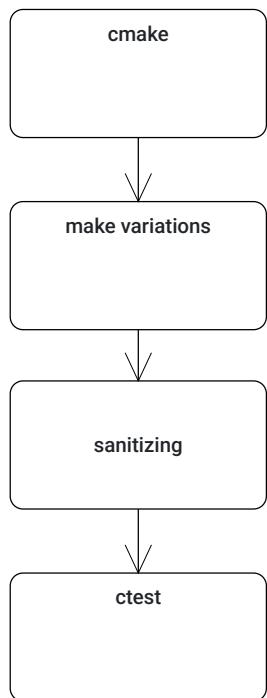
# The problem

1. Outer boxes may not have the expected sidelengths
2. Interacting with neighbouring cells  $\Rightarrow$  Catching everything in  $r_{cutoff}$



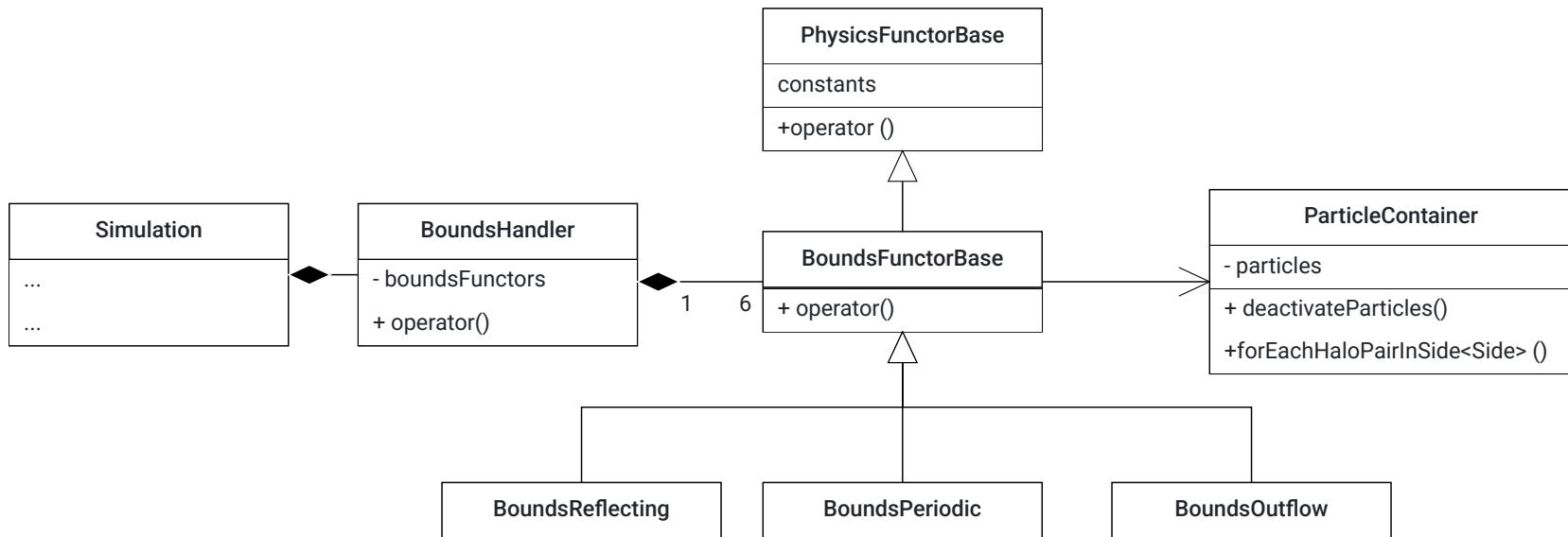
$\Rightarrow$  Interact with one more „Cellblock“ in that direction

# CI/CD improvements

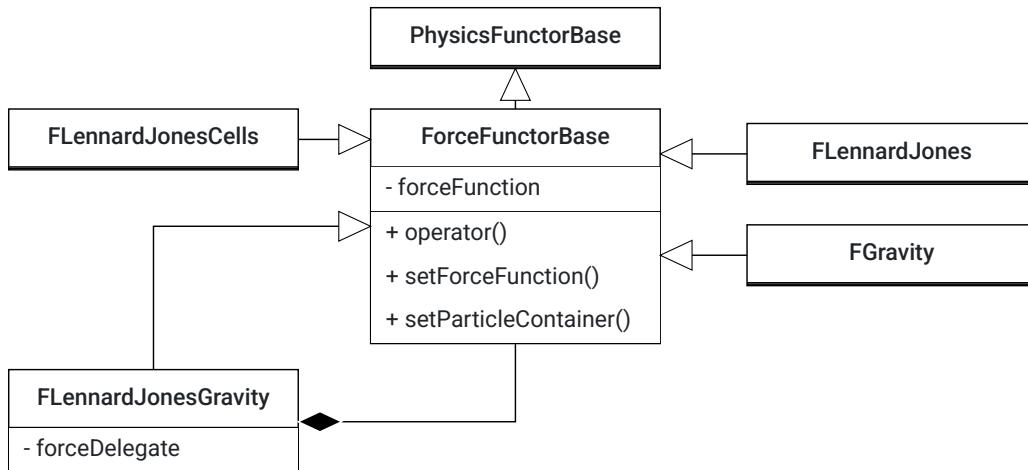


# Adding Periodic bounds

This slide should look very familiar to Assignment 3

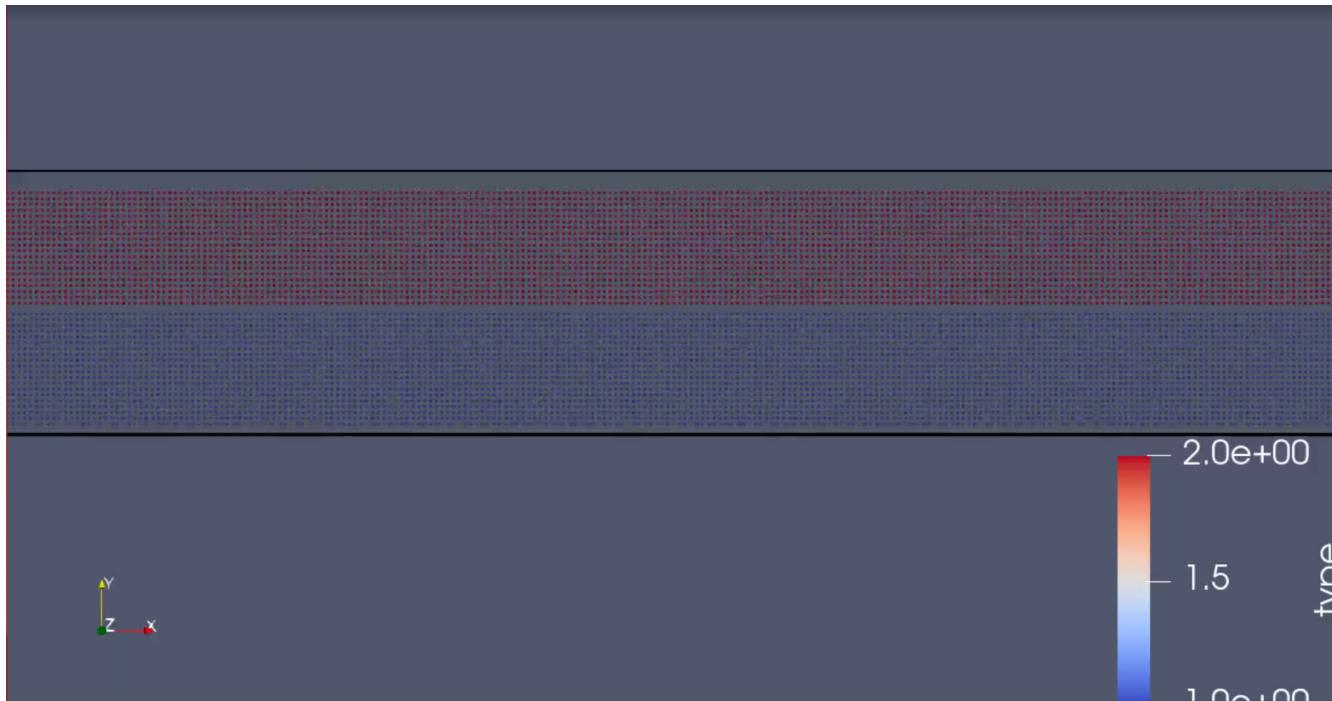


# Adding Gravitational Force

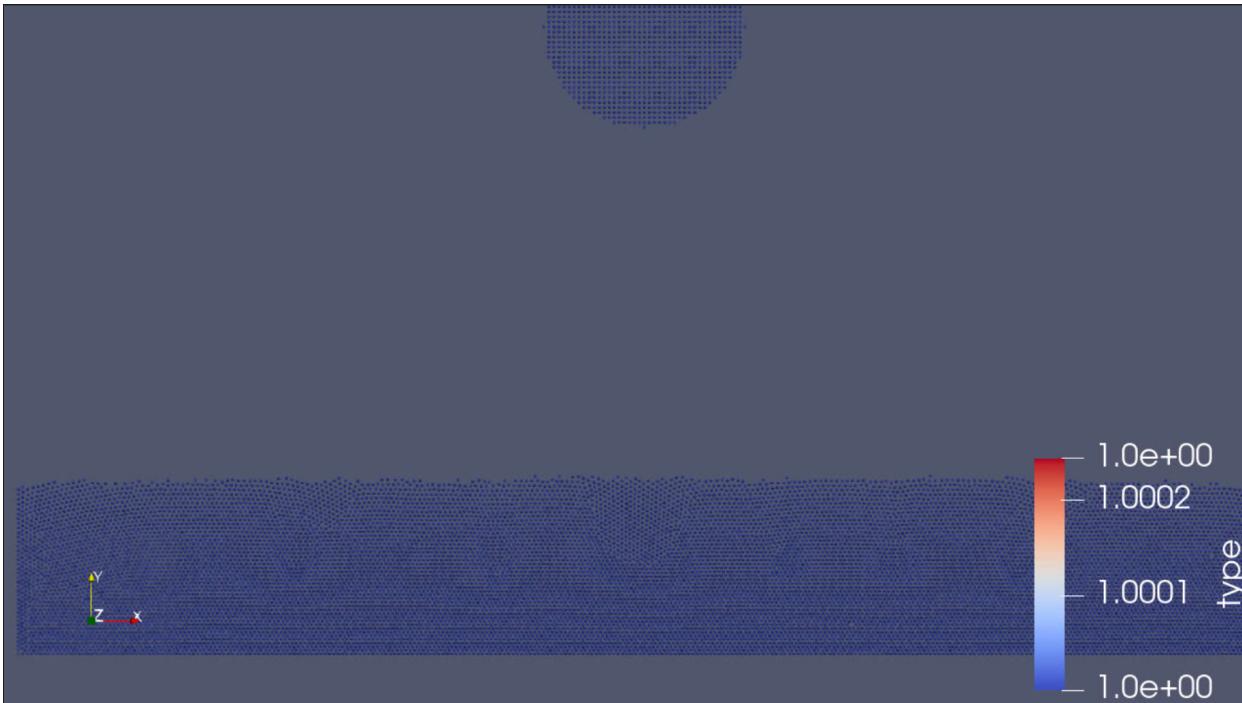


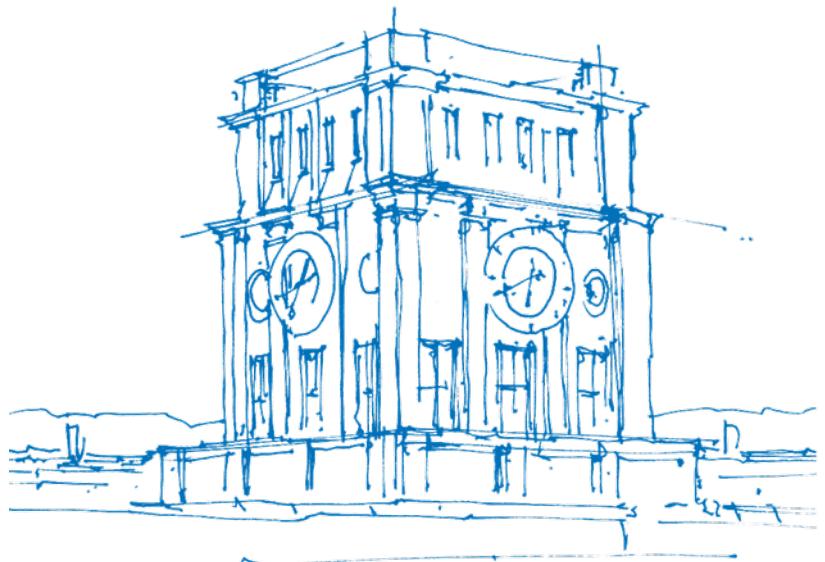
```
FLennardJonesGravity :: operator ()(){
    forceDelegate->operator ();
    particleContainer.forAllParticles ([]( auto& p){
        p.force[1] += p.m * gGrav;
    });
}
```

# Rayleigh-Taylor instability



# Falling drop





TUM Uhrenturm