Molecular Dynamics - Assignment 4

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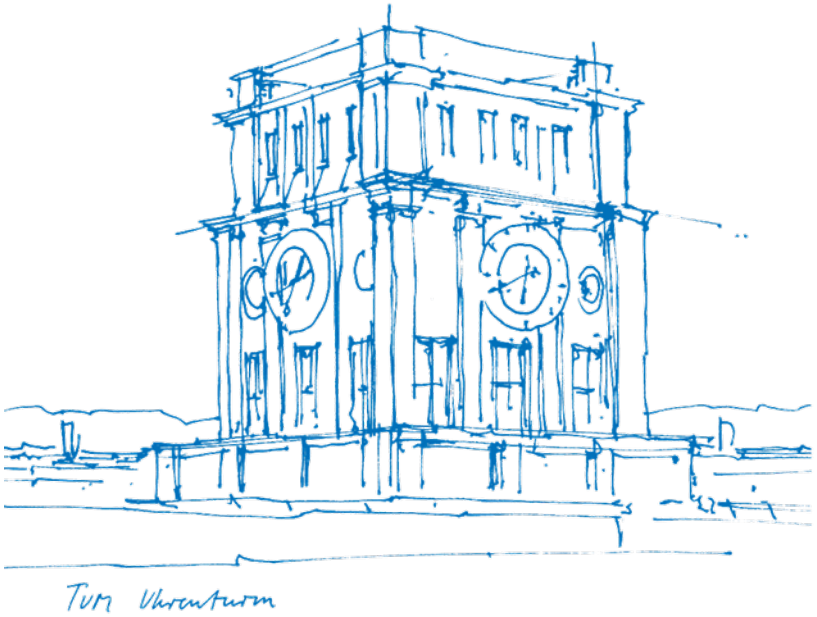
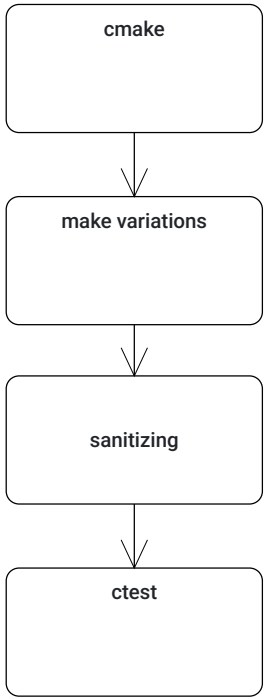
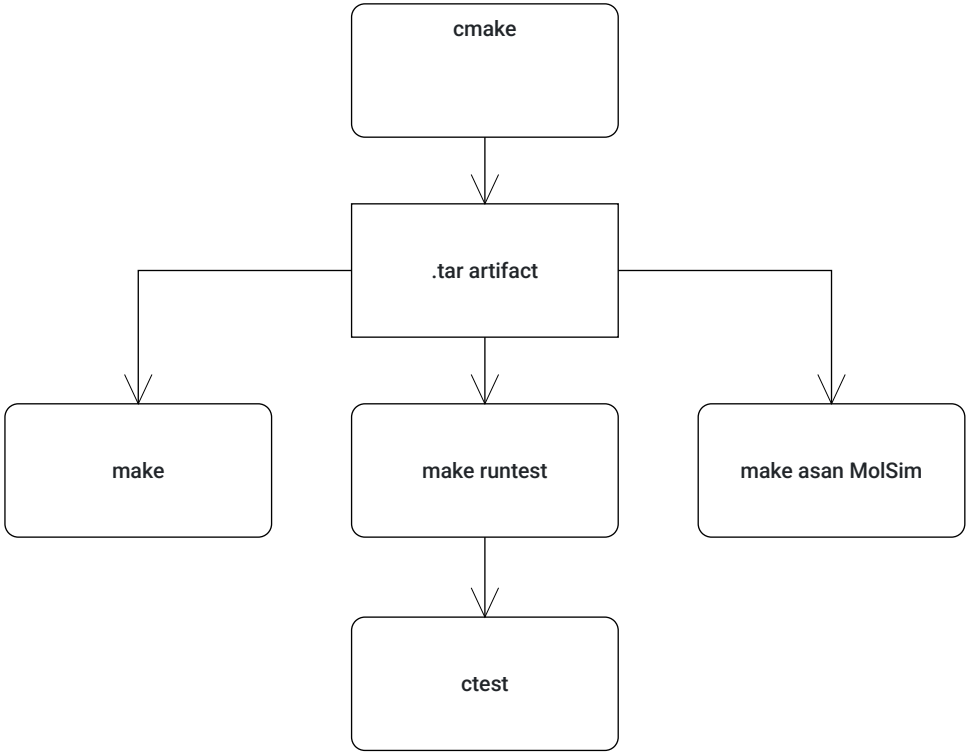


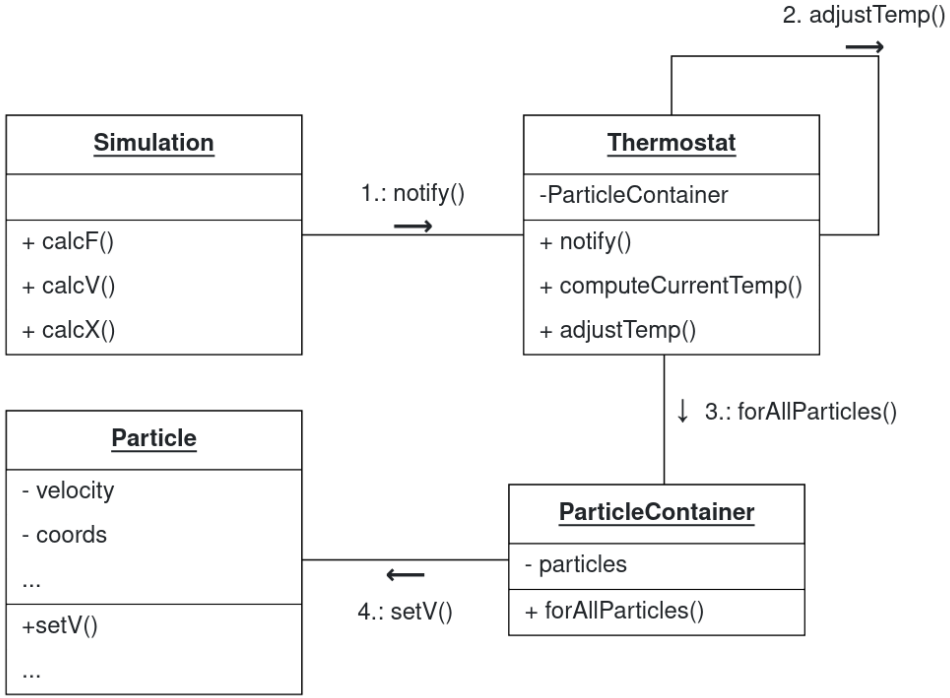
CI/CD improvements





Reduced CI/CD time from 5m30s to 3m

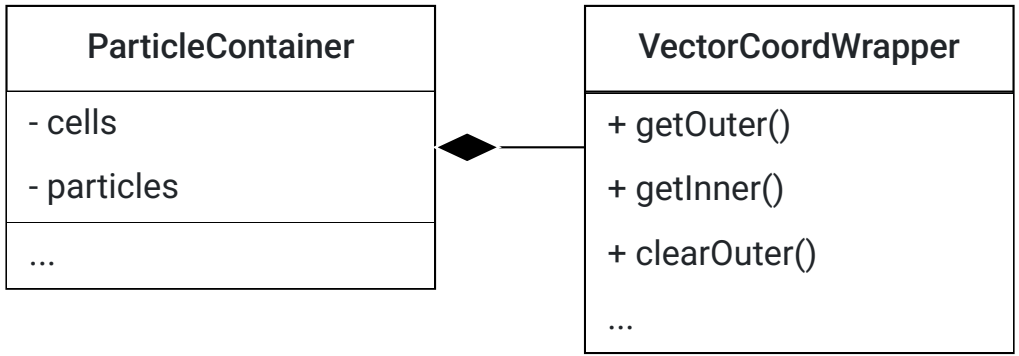
Thermostat

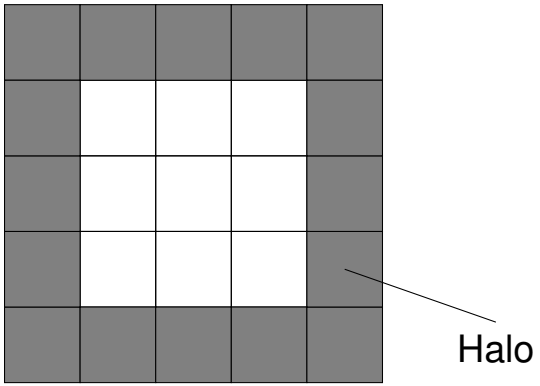

2. adjustTemp()
Simulation
+ calcF()
+ calcV()
+ calcX()
1.: notify()
Thermostat
-ParticleContainer
+ notify()
+ computeCurrentTemp()
+ adjustTemp()
3.: forAllParticles()
Particle
- velocity
- coords
...
+setV()
...
4.: setV()
ParticleContainer
- particles
+ forAllParticles()

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

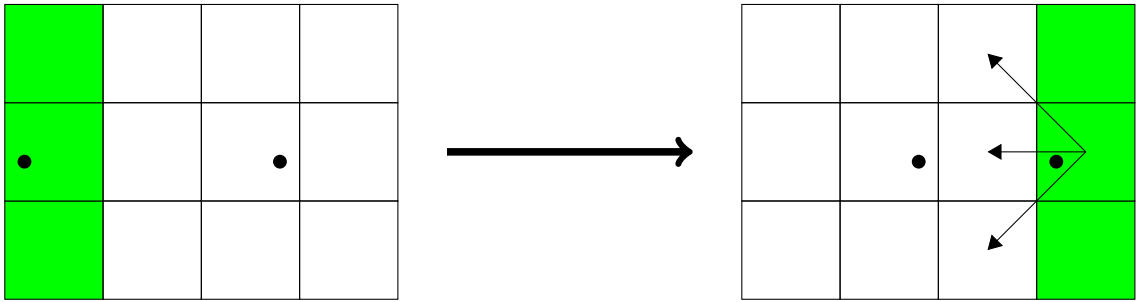




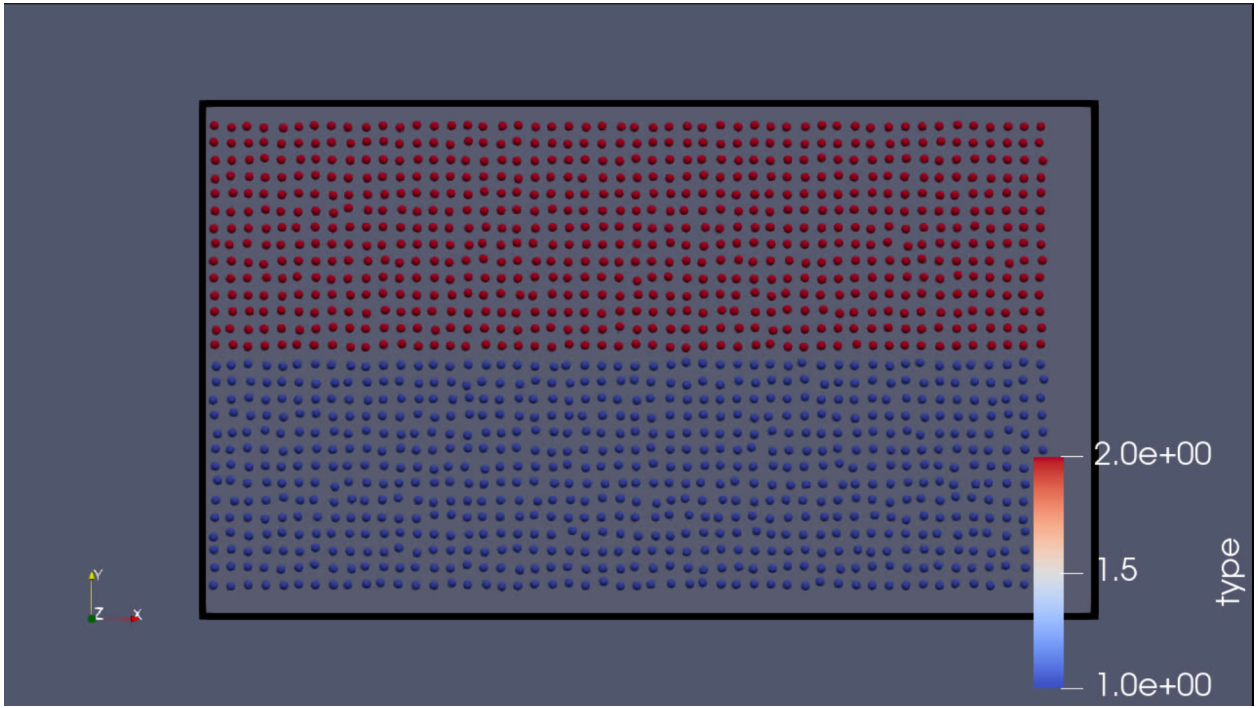
Boundary conditions

Idea:

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

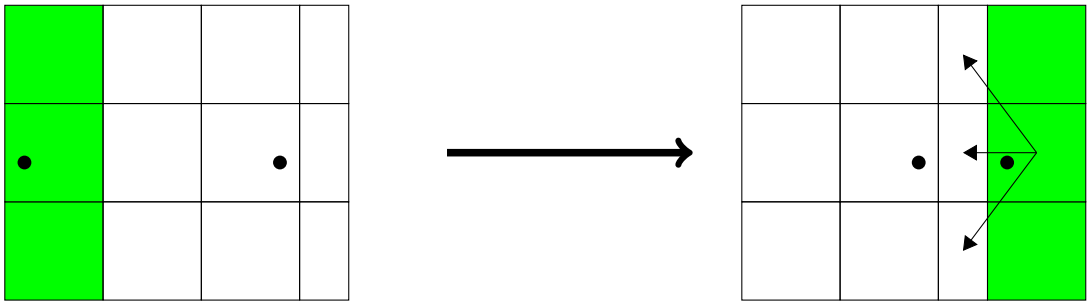


The result



The problem

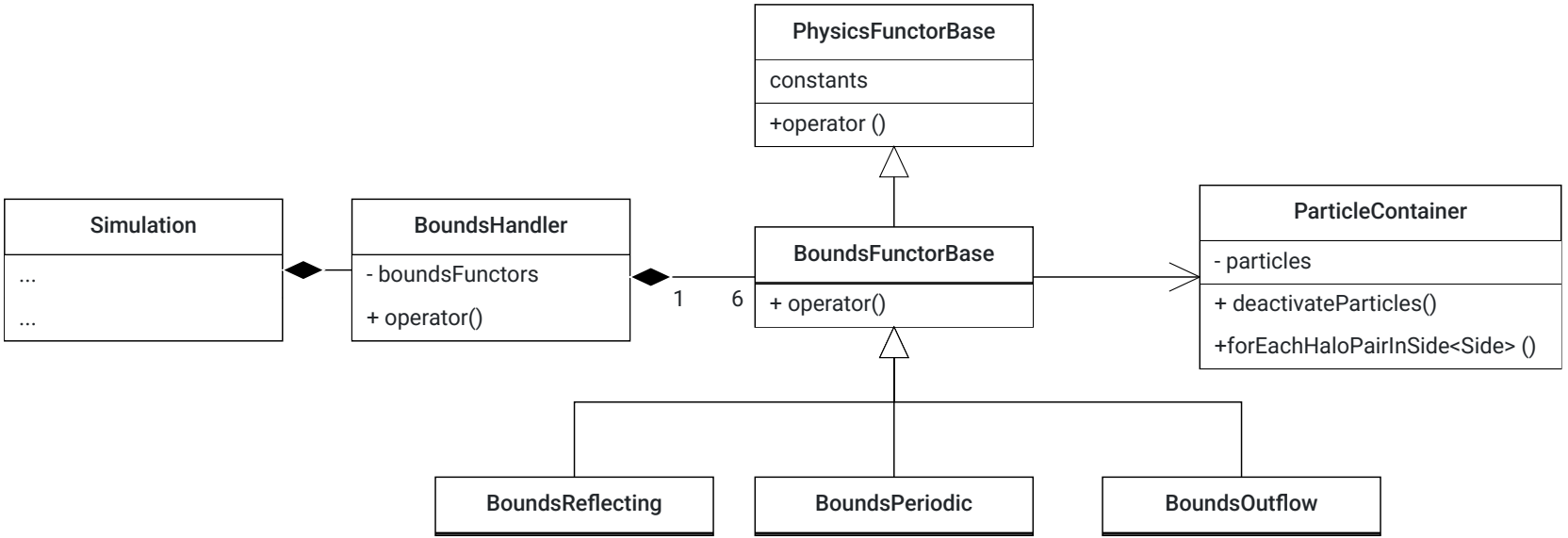
1. Outer boxes may not have the expected sidelengths
2. Interacting with neighbouring cells $\not\Longrightarrow$ Catching everything in r_{cutoff}



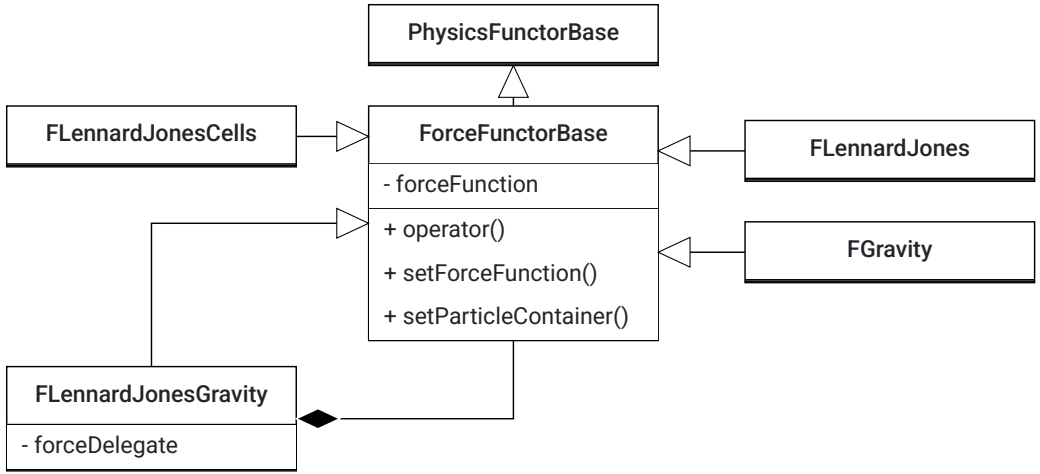
$\Longrightarrow$ Interact with one more „Cellblock“ in that direction

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;
        });      }
```

Optimizations 1

As mentioned in Assignment 3 our ParticleContainer does not contain Particle-structs anymore. Keeping the old interface lead to the following method:

```
void ParticleContainer::forAllParticles(void(*function)(Particle &)) {
        for (unsigned long index: activeParticles) {
                Particle p;
                loadParticle(p, index);
                function(p);
                storeParticle(p, index);
        }
}
```

$\Longrightarrow$ rewriting old code where this method got used was a major improvement

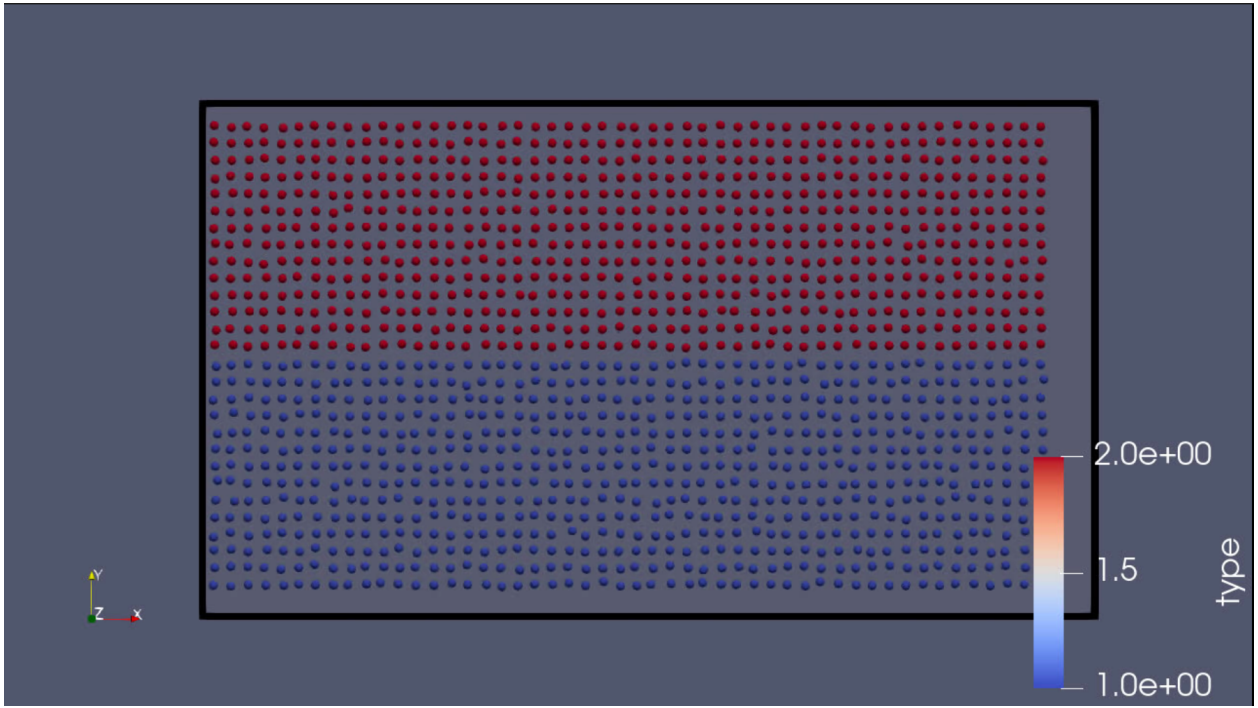
Optimizations 2

▼ sim::Simulation::runBenchmark	100.0%	0s	MolSim	sim::Simulati…		0x63282
▼ sim::physics::force::FLennardJonesCells::operator()	88.2%	0s	MolSim	sim::physics:…		0x143b94
▼ ParticleContainer::forAllDistinctCellNeighbours<sim::physics::force::FL	81.6%	0.024s	MolSim	ParticleCont…		0x143dd6
▶ sim::physics::force::FLennardJonesCells::operator()(void)::{lambda(s	80.9%	0.640s	MolSim	sim::physics:…		0x143a00
▶ ParticleContainer::VectorCoordWrapper::operator[]	0.4%	0.012s	MolSim	ParticleCont…		0x76be6

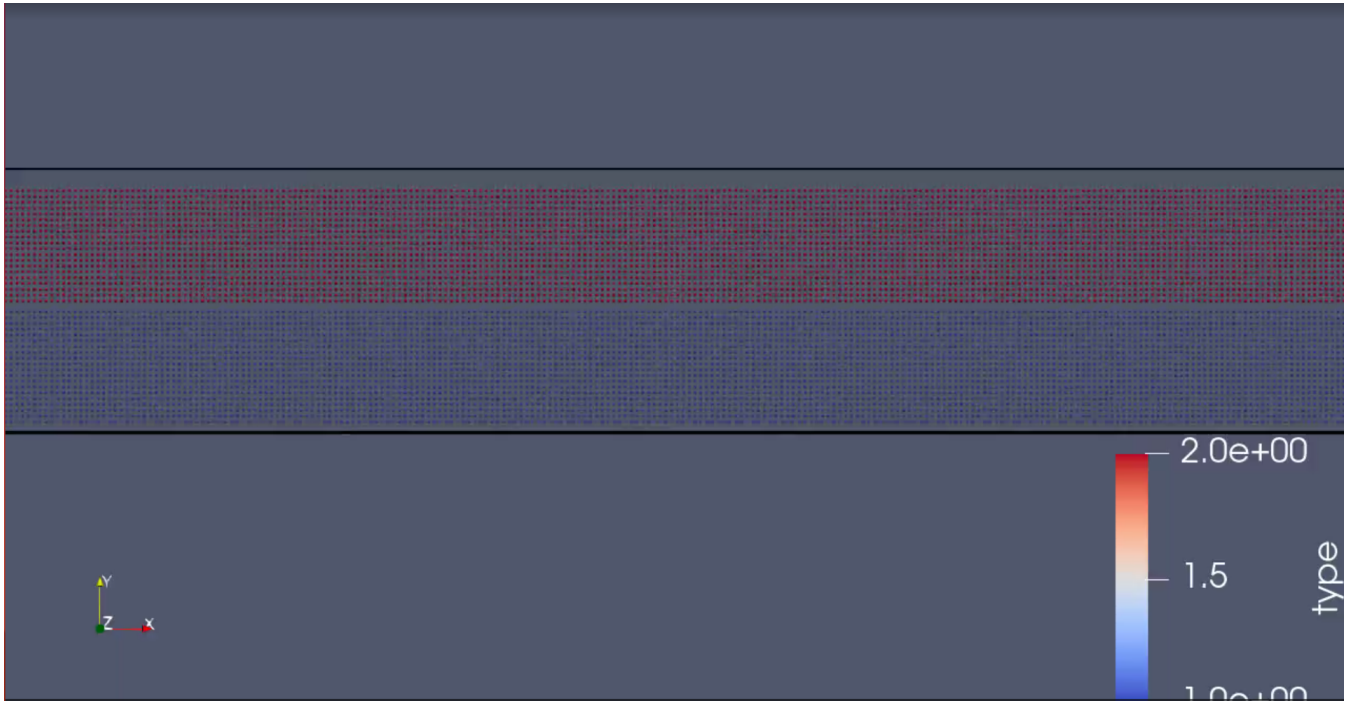
- Force calculation takes a significant portion of CPU time
- Force between two particles in Force-Functors got represented as lambda expression

$\Longrightarrow$ Represent force as static function instead

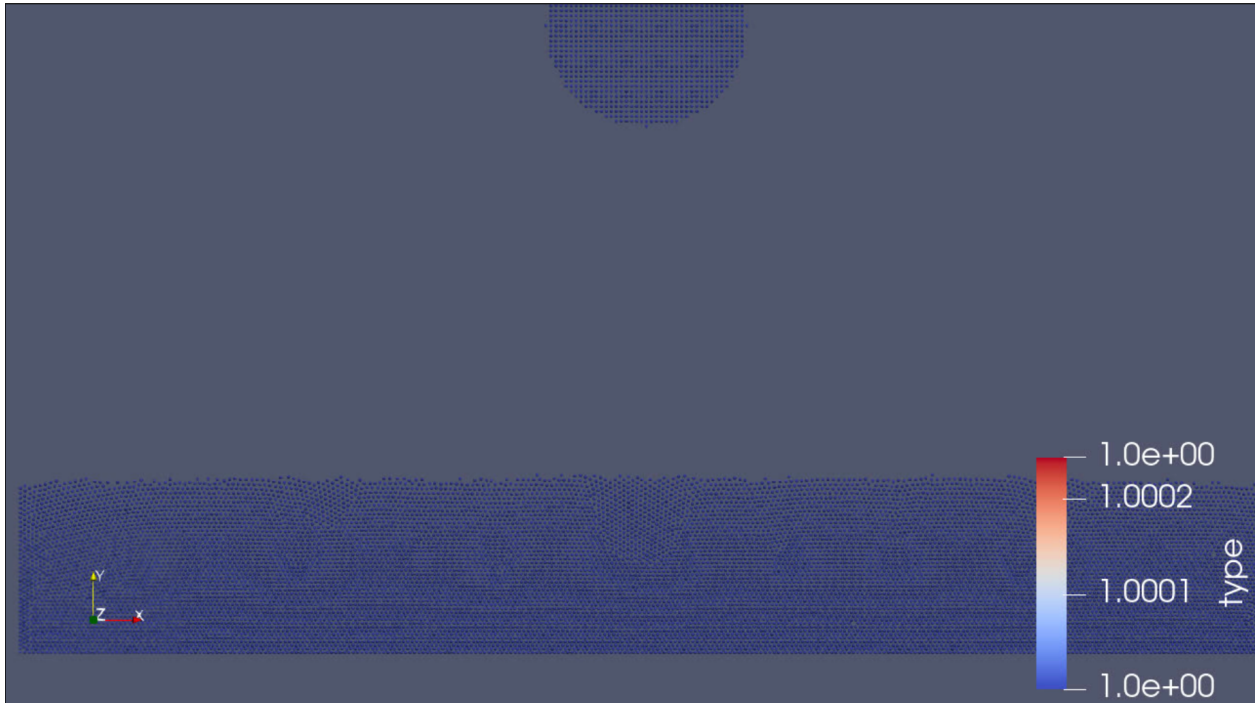
Small Rayleigh-Taylor instability



Rayleigh-Taylor instability



Falling drop



Serial Benchmarks

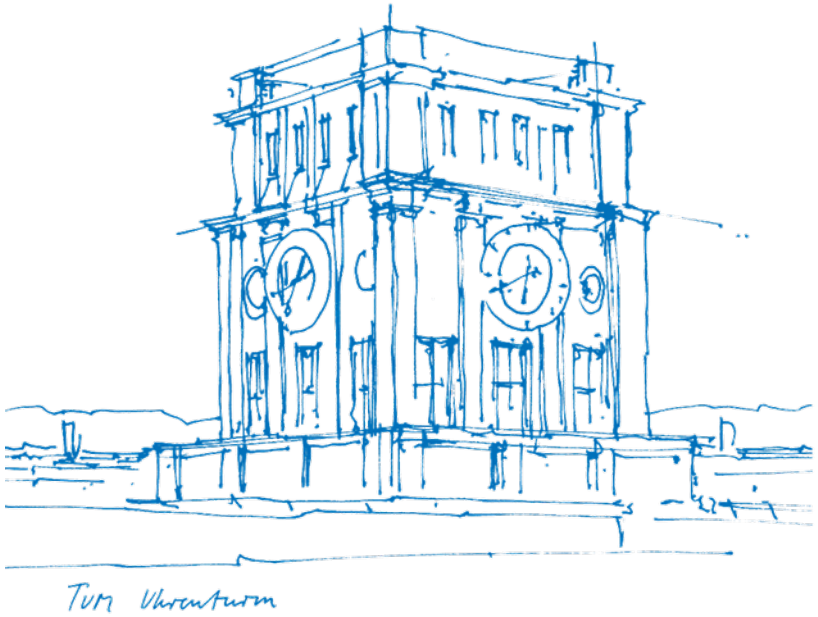
- As already mentioned building with the Intel compiled didn't work even with major time investments
- The option „-slow“ lets the code run in the pre-optimized state

Options	MMU/s Cluster	MMU/s Local
-slow -O2	0.0087	$\geq 1/6 \cdot 0.036 \wedge \leq 1/2 \cdot 0.036$
-O2	0.0087	0.036
-O0	0.0087	0.036

Since these measurements are so close together and significantly smaller than our local measurements, we assume that something went wrong on the cluster.

Roadblocks

- Compiling and running jobs on the cluster turned out to be a nightmare
- Intel compiler broke us trying to unbreak him
- Searching for bugs that may or may not be there (bouncy particles in Rayleigh-Taylor)
- Searching for bugs that definitely are there (see Boundary conditions)
- Large time investments in order to get tools to run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Recreating Profiling

1. `mkdir build`
2. `cmake ..`
3. `make ProfileMolSim` or `make CXX_FLAGS+=Dslow -std=c++20"ProfileMolSim`
4. `./ProfileMolSim ../input/[file_you_want_to_profile]`
5. `gprof ProfileMolSim gmon.out > profile-data.txt`