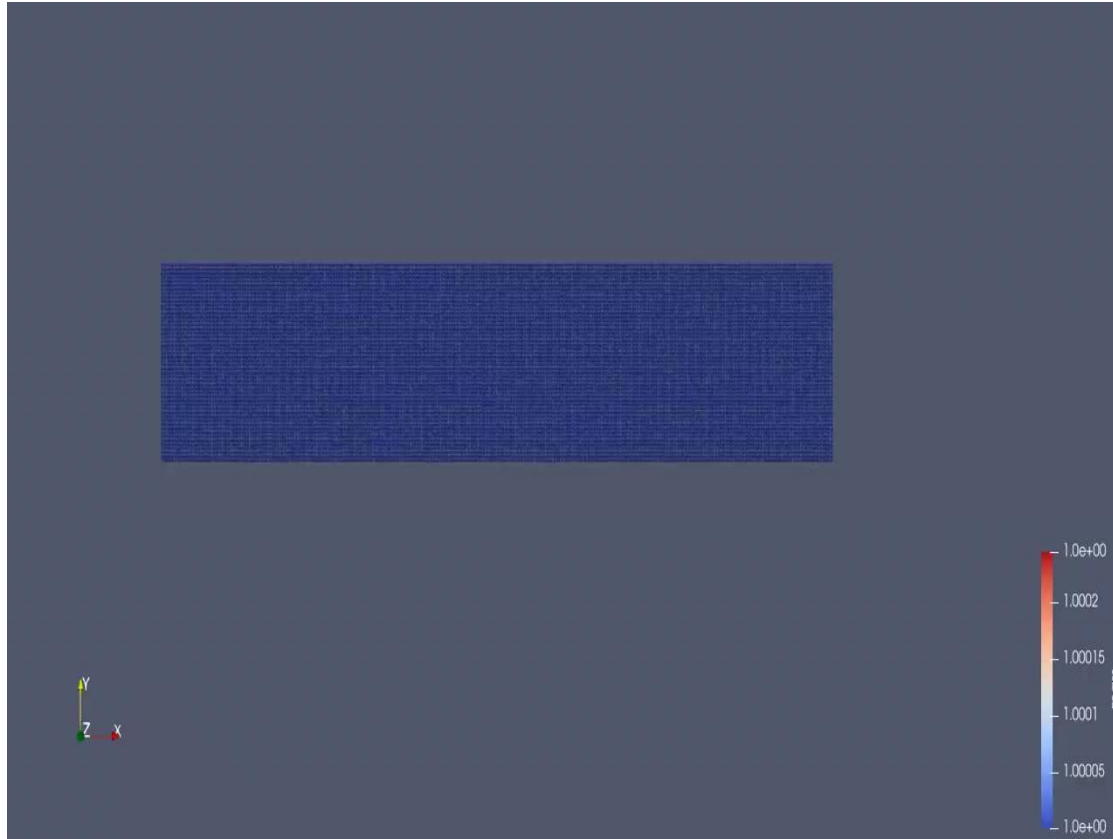


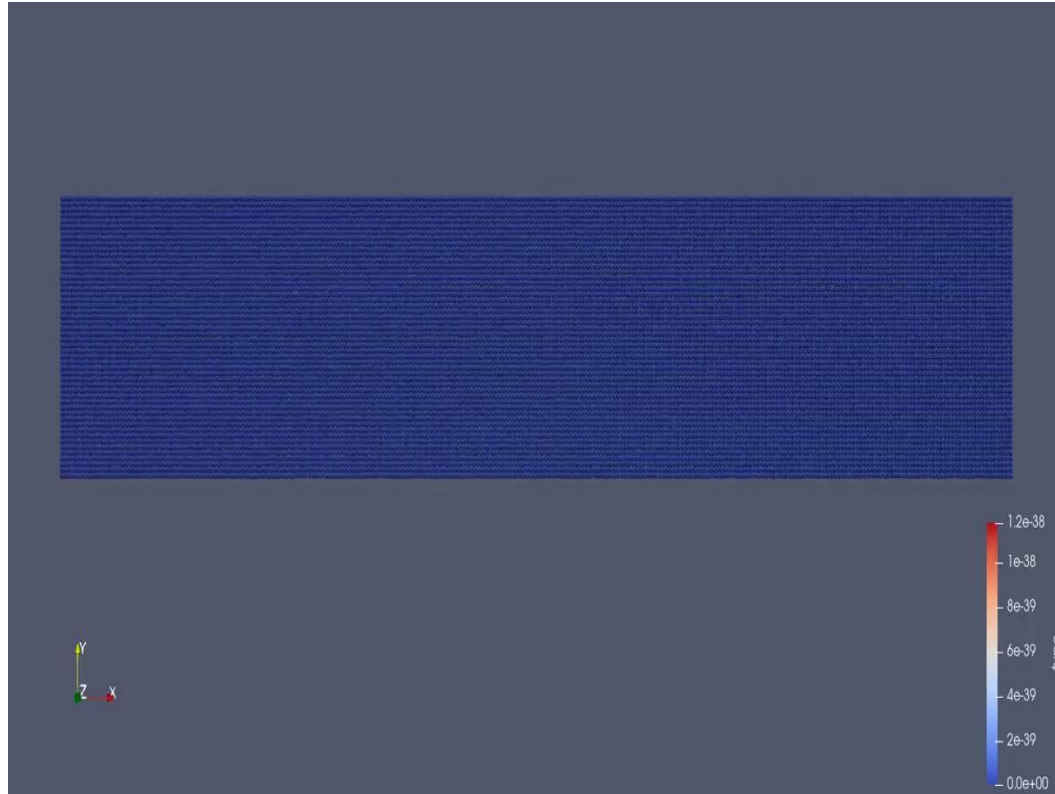
# Worksheet 4

Thermostats, Rayleigh-Taylor instability  
and “falling drops”

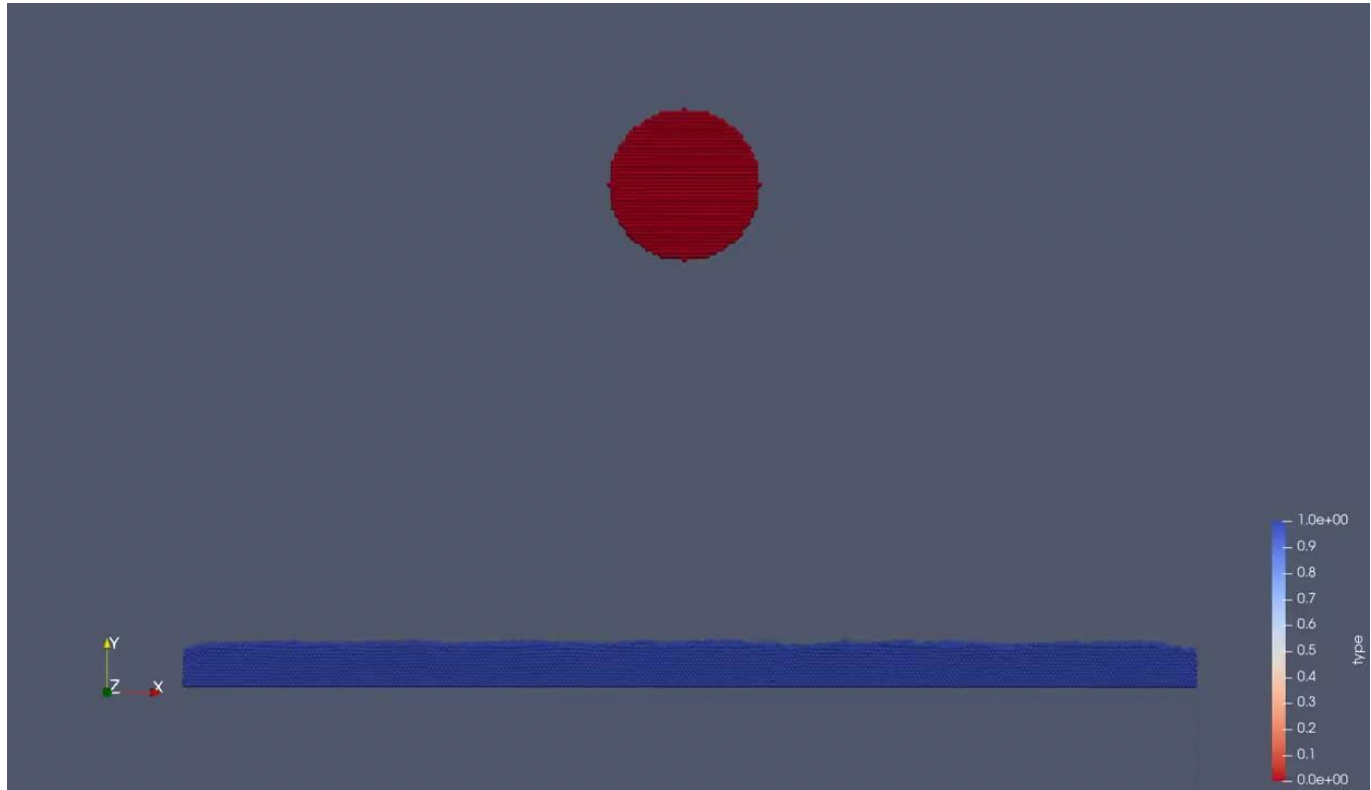
# Fluid Equilibration



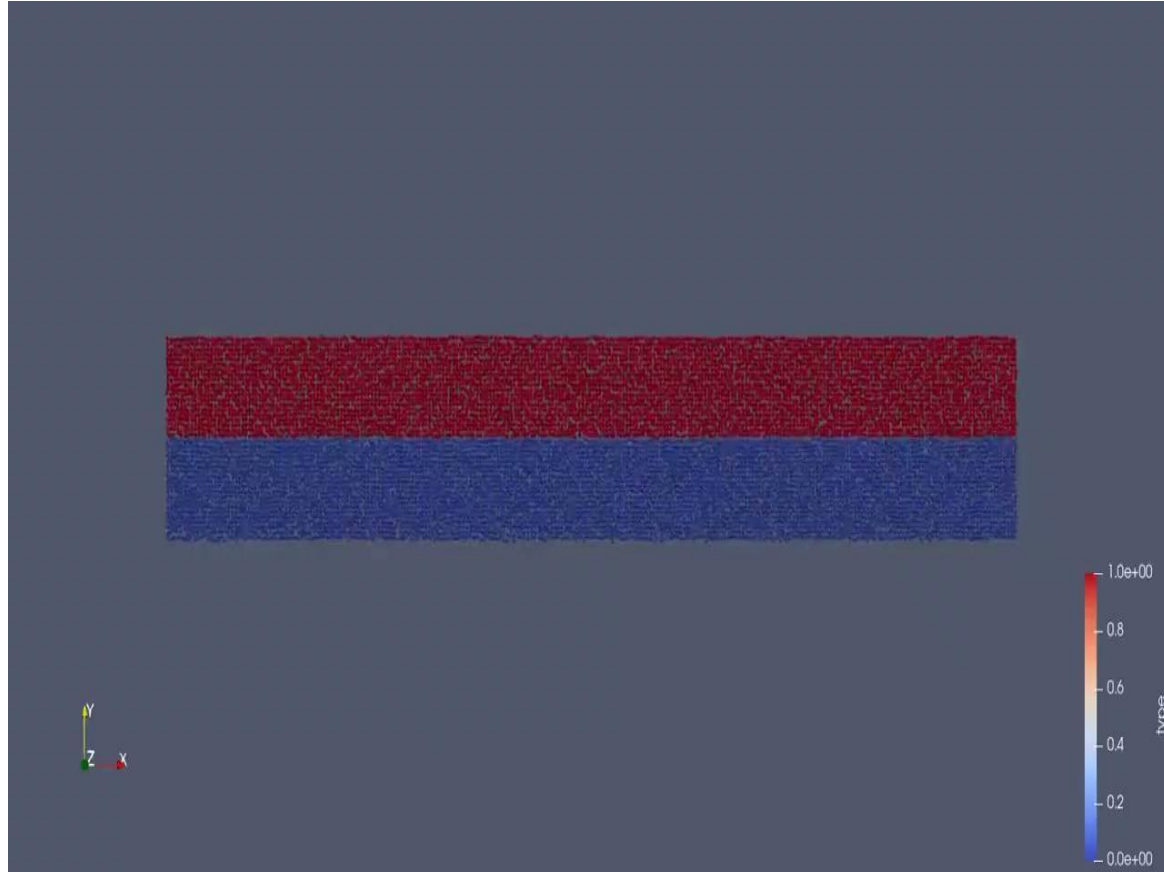
# Water on the moon?



# How did the universe started?



# Fluid Symphony: Exploring Rayleigh-Taylor Instability



# Profiling

10,38%	MolSim	MolSim	[.] std::__array_traits<double, 3ul>::_S_ref
9,65%	MolSim	MolSim	[.] std::array<double, 3ul>::operator[]
7,75%	MolSim	MolSim	[.] std::array<double, 3ul>::operator[]
5,04%	MolSim	MolSim	[.] operator-
4,47%	MolSim	MolSim	[.] VectorDouble3::VectorDouble3
4,10%	MolSim	MolSim	[.] LinkedCellContainer::applyToPairs
3,76%	MolSim	MolSim	[.] VectorDouble3::getL2Norm
2,73%	MolSim	MolSim	[.] LinkedCellContainer::getGridIndex
2,44%	MolSim	MolSim	[.] LennardJones::CalculateForces
2,37%	MolSim	MolSim	[.] std::array<int, 3ul>::operator[]
2,00%	MolSim	MolSim	[.] std::__array_traits<int, 3ul>::_S_ref
1,78%	MolSim	MolSim	[.] operator+
1,74%	MolSim	MolSim	[.] LinkedCellContainer::getParticleIndex
1,47%	MolSim	MolSim	[.] std::array<double, 3ul>::size
1,46%	MolSim	libm.so.6	[.] __sqrt_finite@GLIBC_2.15
1,42%	MolSim	MolSim	[.] LinkedCellContainer::applyToAll
1,42%	MolSim	MolSim	[.] operator*
1,38%	MolSim	MolSim	[.] std::operator!=
1,35%	MolSim	MolSim	[.] std::__cxx11::list<Particle, std::allocator<Particle> >::begin
1,26%	MolSim	MolSim	[.] std::_List_iterator<Particle>::_List_iterator
1,22%	MolSim	MolSim	[.] std::__cxx11::list<Particle, std::allocator<Particle> >::end
1,05%	MolSim	MolSim	[.] Particle::getXVector

# Thermostat optimization

- ***Problem:*** the state of the thermostat is updated in each iteration - two copies of all particles per iteration
- ***Solution:*** only update state when thermostat is actually used
- ***Results:*** no difference, regardless of compiler optimization level, regardless of frequency of thermostat

# Particle optimization with VectorDouble

- ***Problem:*** particle attributes stored as VectorDouble, most used getters and setters use VectorDouble - many std::array and VectorDouble constructions
- ***Solution:*** store Particle attributes as VectorDouble
- ***Results:*** ca 10% execution time decrease



# Lookup table for getGridIndex

- ***Problem:*** function called many times for the same values in LinkedCellContainer
- ***Solution:*** precalculate values and use a lookup-table
- ***Results:*** no difference, probably due to getGridIndex not taking that much time in total compared to the rest of the simulation

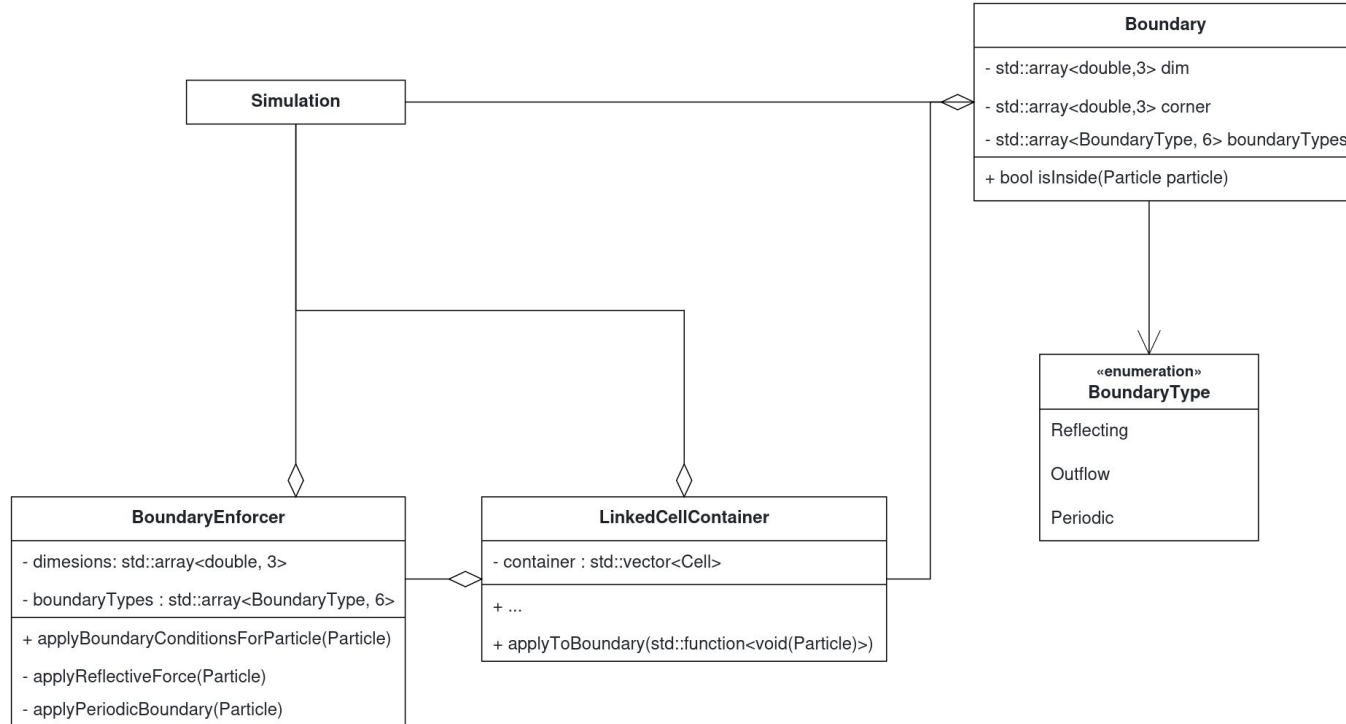
# SIMD for VectorDouble

- ***Problem:*** we call VectorDouble operators (+, -, \*) very often per iteration
- ***Solution:*** use SIMD instructions to do all three calculations at once
- ***Results:*** no difference - SIMD overhead, other parts of the program take more time

## Mixing Rules Optimization: **compute once, reuse anywhere**

- **Problem:** in force calculation, we call `sqrt(p1.getEps() * p2.getEps())`
- **Solution:** store for each particle the value of the square root of Eps and replace the calculation with `p1.getSqrtEps() * p2.getSqrtEps`
- **Results:** no big difference, other parts of the program take more time but this spares a lot of computations

# Implementing boundaries



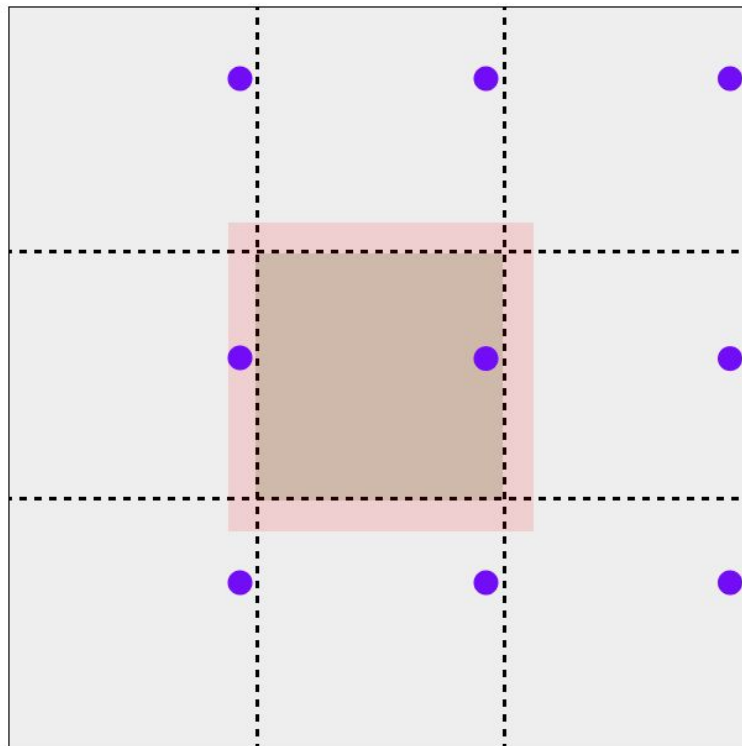
# The periodic boundary

## Principle for Mirroring

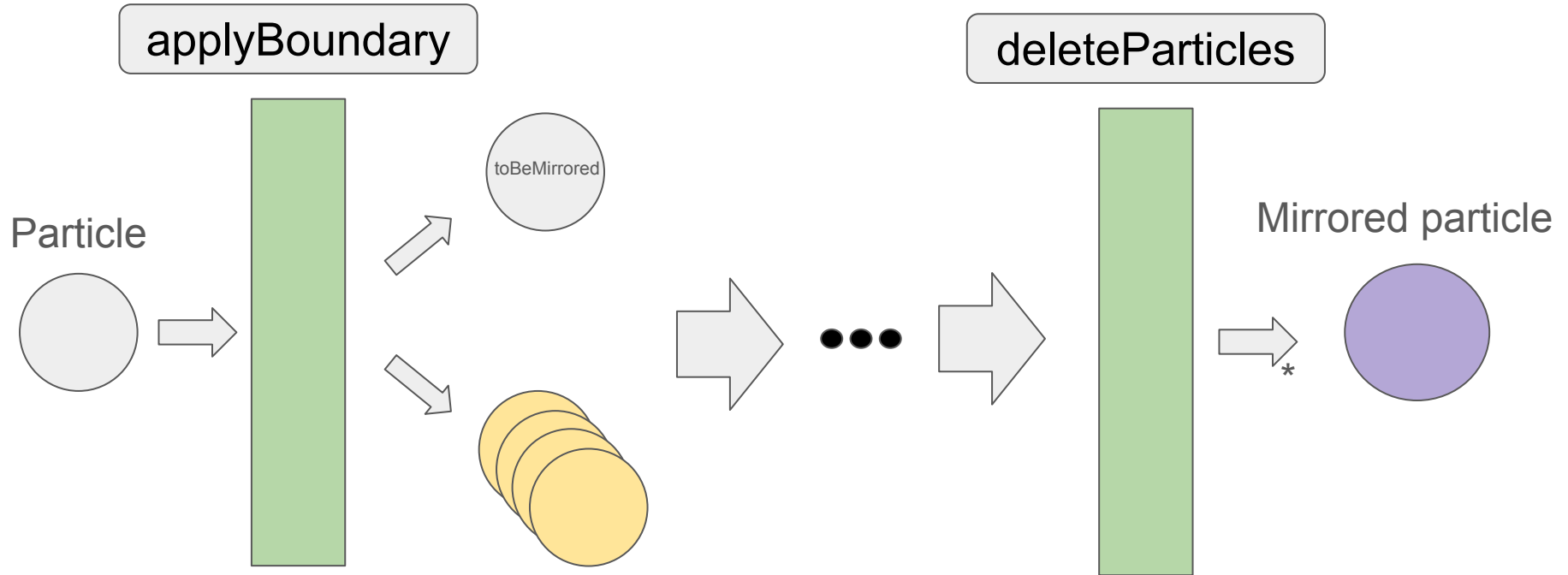
- 1 : Shifting the domain
- 2 : Intersecting with halo region

## Principle for Reinserting

- 1 : Delete old particle
- 2 : Reinsert in opposite side



# Particle Lifecycle - Periodic



\* if particle goes out of bounds