Molecular Dynamics - Assignment 3

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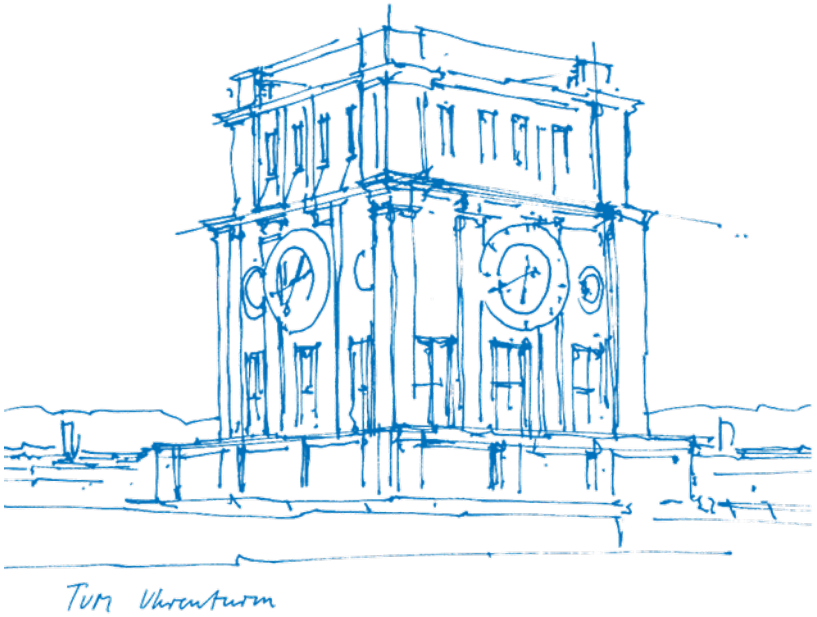
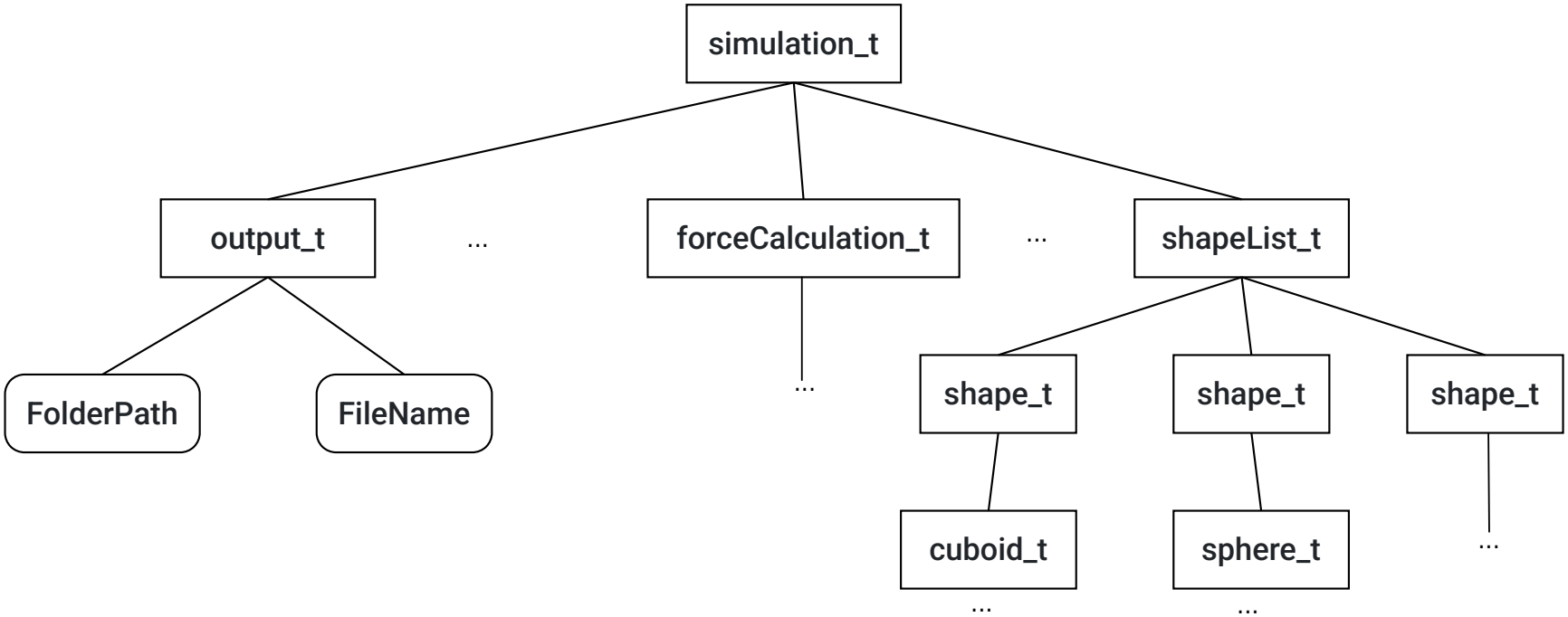
8. Dezember 2022



XSD- tree-like definition of Datastructures



XSD- Code Snippet

- simulation_t stores all the necessary parameters
- Definition utilizes other Datastructures with tree-like definitions
- “simulation_t is root“

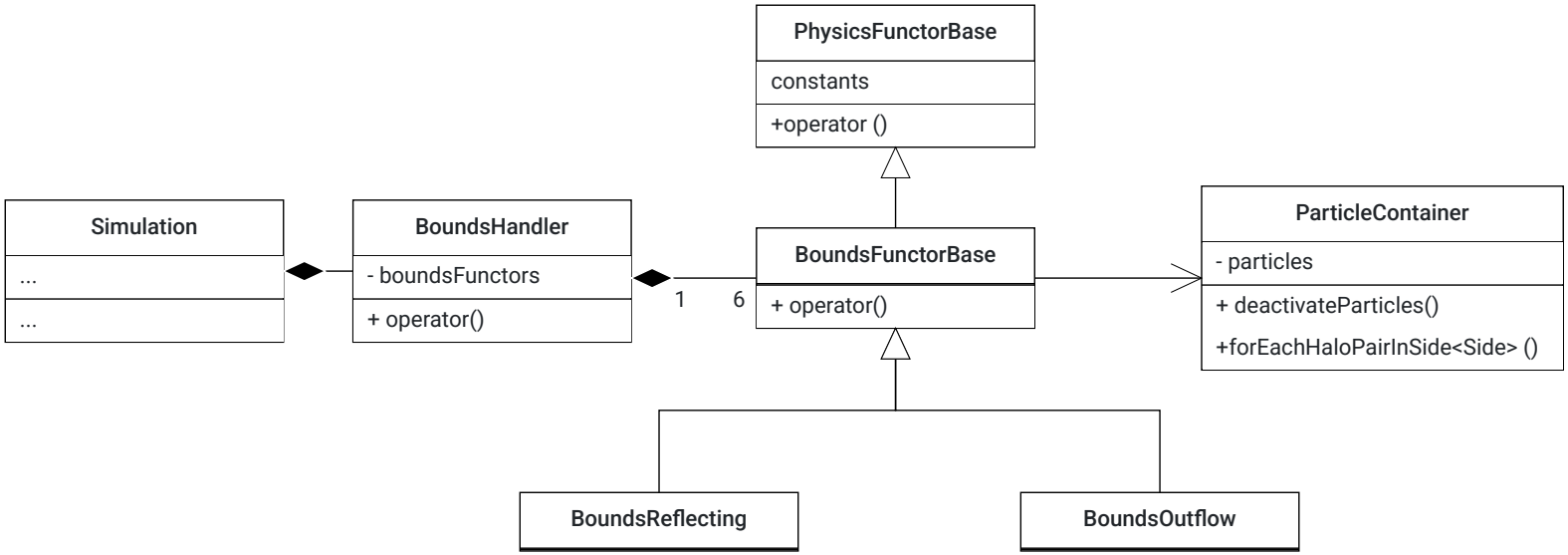
```
<xsd:complexType name="simulation_t">
        <xsd:sequence>
                <xsd:element name="OutputFile" type="output_t" minOccurs="0"/>
                ...
                <xsd:element name="ShapeList" type="shapeList_t"/>
        </xsd:sequence>
</xsd:complexType>
```

XSD- Code Snippet

Trade-Off convenience $\leftrightarrow$ complexity in action:

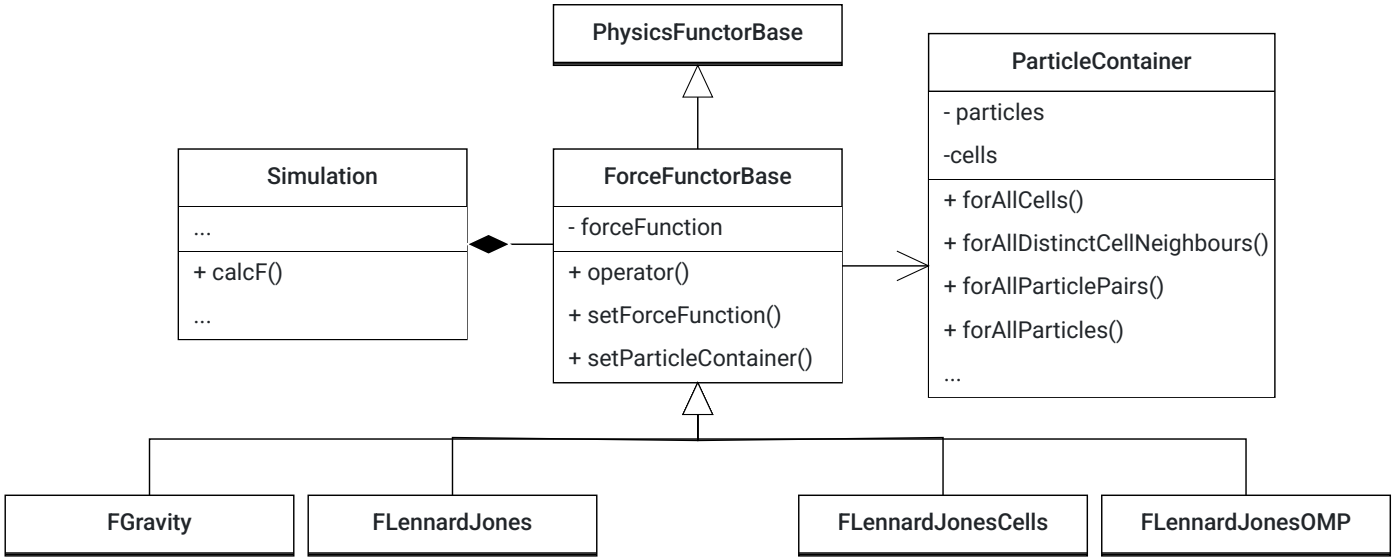
```
<xsd:complexType name="shape_t">
        <xsd:choice>
                <xsd:element name="Particle" type="particle_t"/>
                <xsd:element name="Cuboid" type="cuboid_t"/>
                <xsd:element name="Sphere" type="sphere_t"/>
        </xsd:choice>
</xsd:complexType>
```

Bounds Handling



ForceFunctors

- Force function used gets determined on runtime via input parameters
- Force functor defines the algorithm (Linked-Cell algorithm/ All-Pairs algorithm) used

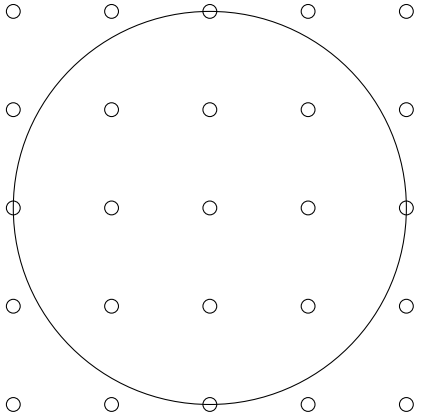


Spheres

Expansion of the Body-struct utilized in Assignment 2

```
enum Shape {cuboid, sphere};
struct Body {
        Shape shape;
        Eigen::Vector3d fixpoint;
        Eigen::Vector3d dimensions;
        double distance;
        double mass;
        Eigen::Vector3d start_velocity;
};
```

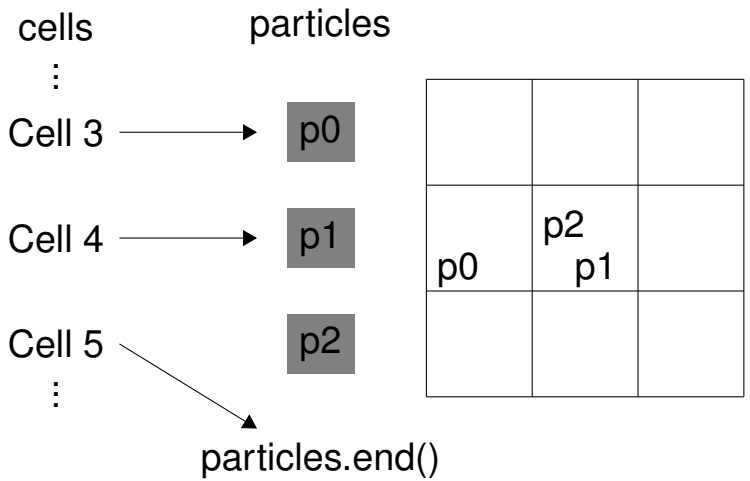
$$\sqrt{x^2 + y^2 + z^2} <= r$$
$$\iff x^2 + y^2 + z^z <= r^2$$



The Cell Data-Structure - Approach 1

Idea:

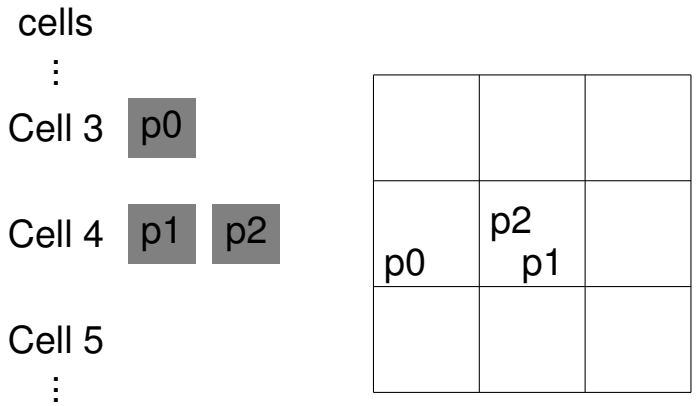
- Sort Particles in accordance to their Cell Position
- save which part of the particles-Vector corresponds to which cell



The Cell Data Structure - Approach 2

Idea:

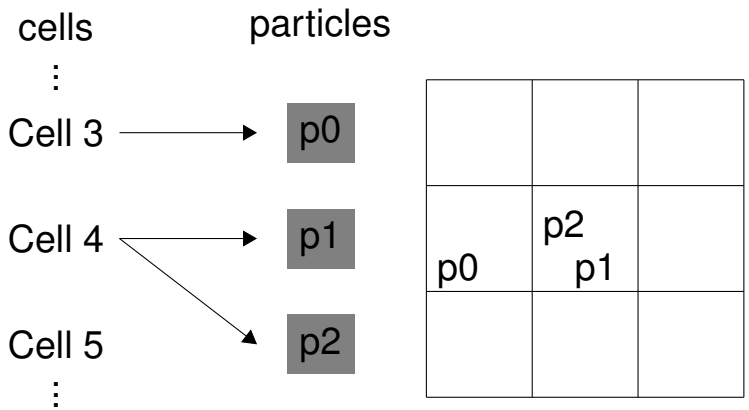
Approach 1.1 stored multiple virtual vectors in one vector $\rightarrow$ let's actually store the particles in vectors corresponding to their cell



The Cell Data Structure - Approach 3

Idea:

- Each Cell only keeps references to their members
- No sorting or copying of entire particles required



Approach Comparison

Approach 1	Approach 2	Approach 3
+ Easy to implement	+ Easy to implement	+ Easy to implement
+ Interface for old Assignments remains unchanged	+ New Implementation of some methods needed	− Interface for old Assignments remains unchanged
− Expensive struct swaps during sorting	− Expensive struct copies with potential reallocs needed	+ References are cheap
+ Direct access to particles for calculations	+ Direct access to particles for calculations	+ Dereferencing needed

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In the end we decided to implement approach 3.

ParticleContainer's new methods

```
class ParticleContainer{
        ...

        void forAllPairsInSameCell(void (*fun) (Particle& p1, Particle& p1));

        void forAllPairsInNeighbouringCell(void (*fun) (Particle& p1, Particle& p1));

        void forAllCells(void (*fun)(...));

        void forAllDistinctNeighbouringCells(void (*fun) (...));

        ...
}
```

- Functionality of first two methods is sufficient but hard to optimize
- Functionality of last two methods results in higher cohesion, but potential for runtime improvement

Runtime measurement setup

- Particles initiated in a square with varying dimensions

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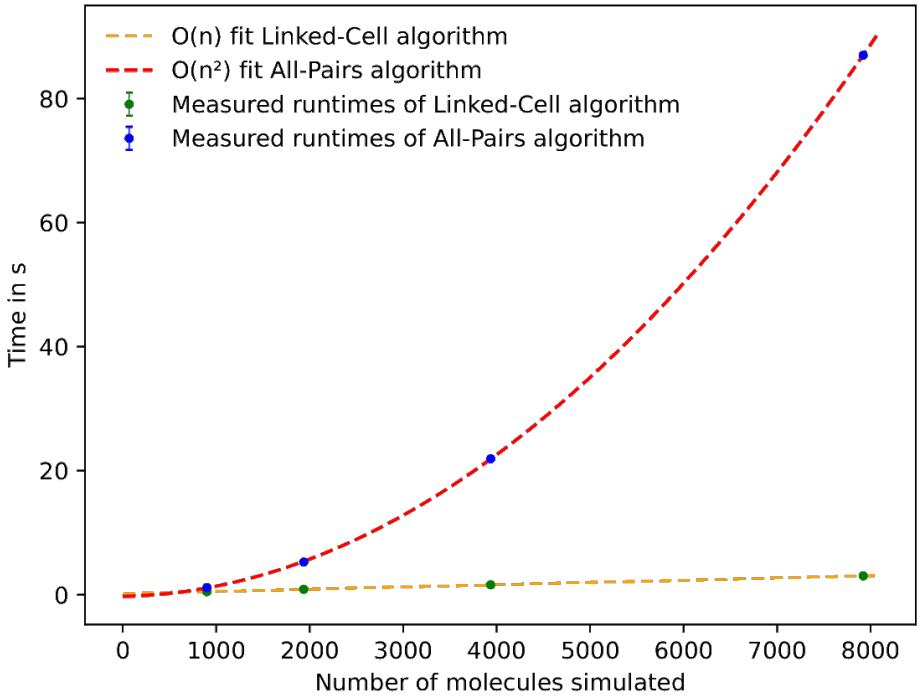
- exact commands to recreate the results are in README and at the end of this presentation

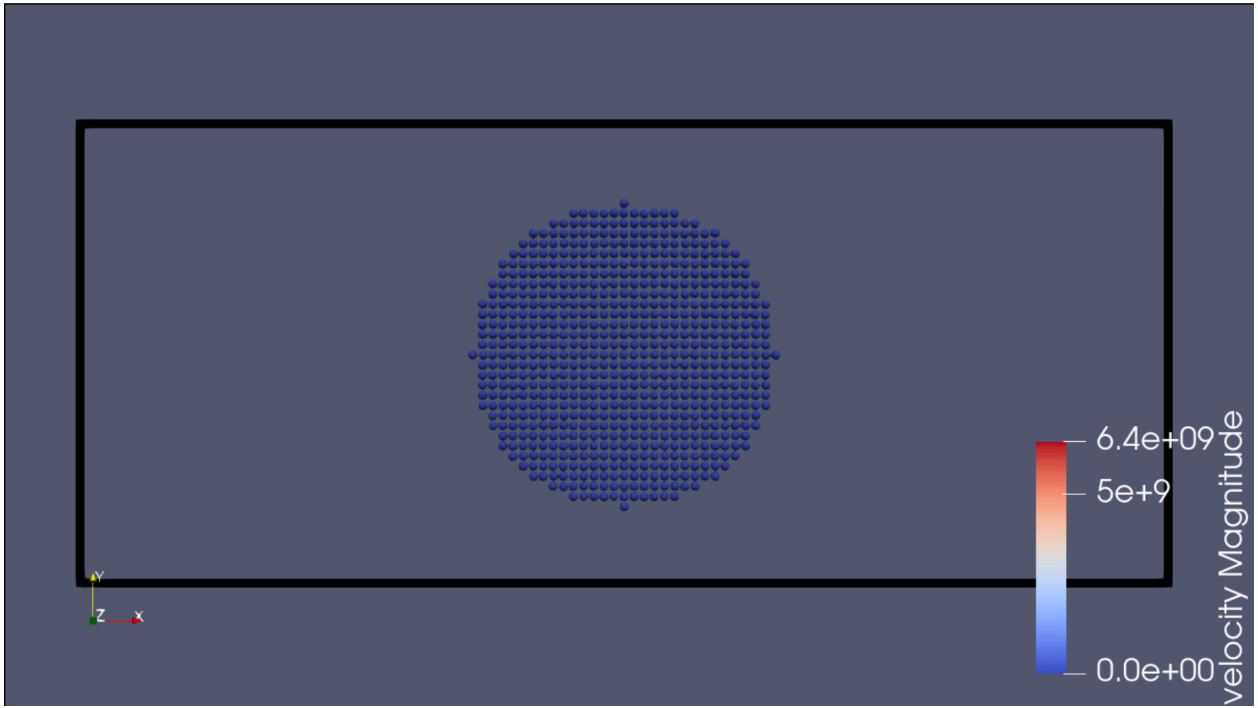
Runtime Comparison of different algorithms



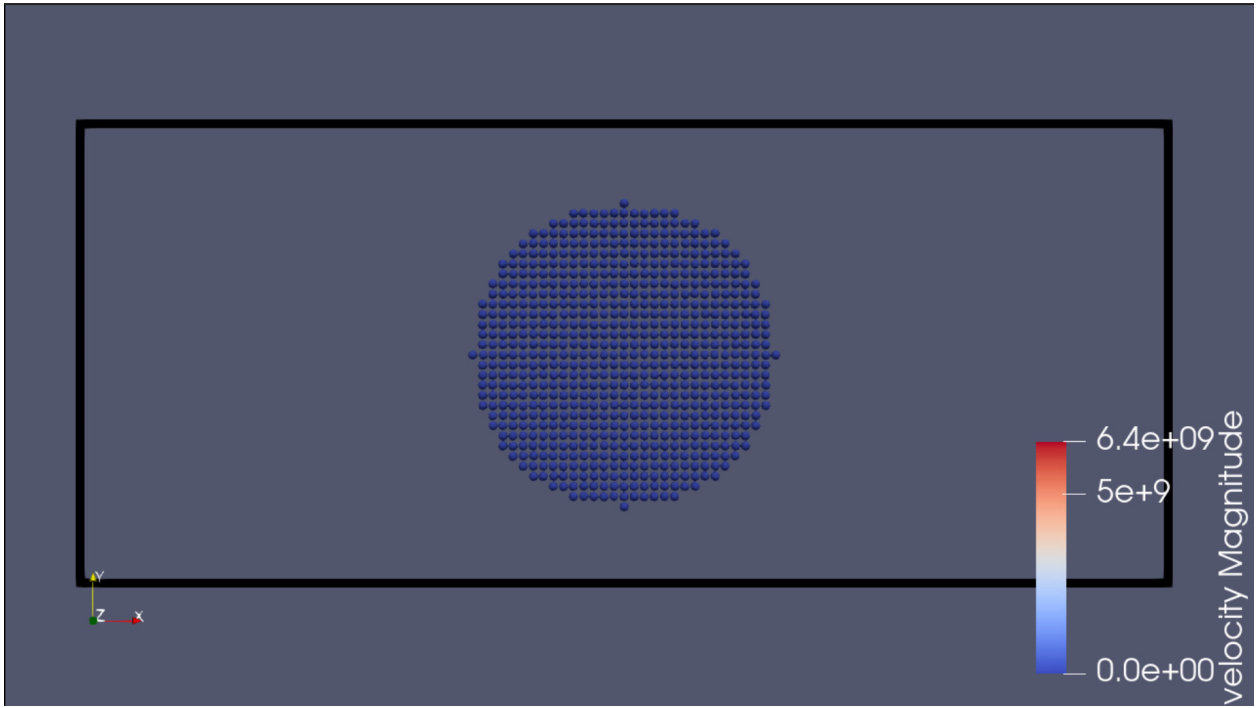
Hardware details:

Ubunutu 20.04 LTS
i7 – 12700KF @5,0GHz
64GB RAM @ 3200MHz

Our Simulation

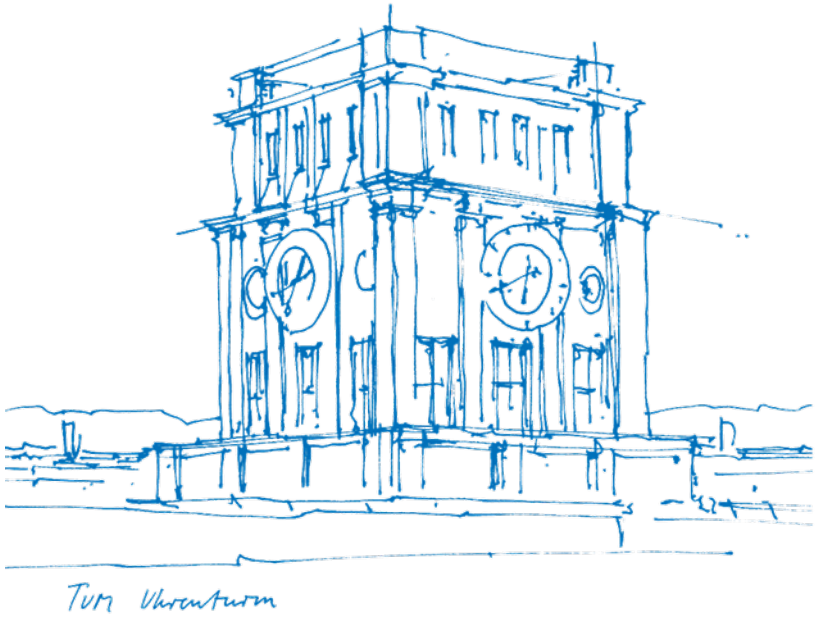


Doubling Δt



Roadblocks and lessons learned

- Play the objective!
- Getting together and figuring out an elegant solution for one hour is an hour well spent
- Clearly define Interfaces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Recreating benchmarks

Setup and compilation:

1. mkdir build output
2. cd build
3. cmake ..
4. make

Example of bechmark commands:
Linked-Cell algorithm:
./MolSim ../input/square1.txt -dt 0.0005 -et 0.5 -lc 1 -bbox0 50.0 -bbox1 50.0 -f lennardjonescell -rc 3.0 -bench file -i 10 > ../output/lc_square1.txt

All-Pairs algorithm:
./MolSim ../input/square1.txt -dt 0.0005 -et 0.5 -lc 0 -bbox0 50.0 -bbox1 50.0 -f lennardjones -rc 3.0 -bench file -i 10 > ../output/ap_square1.txt

Recreating benchmarks

- Results can be found in output-folder
- New benchmark files can be written and executed easily
- for other testsizes change input file, output file and bbox-size accordingly

bbox-sizes needed: (50,50), (64,64), (83,83), (109,109)