# Week 1 Molecular Dynamics

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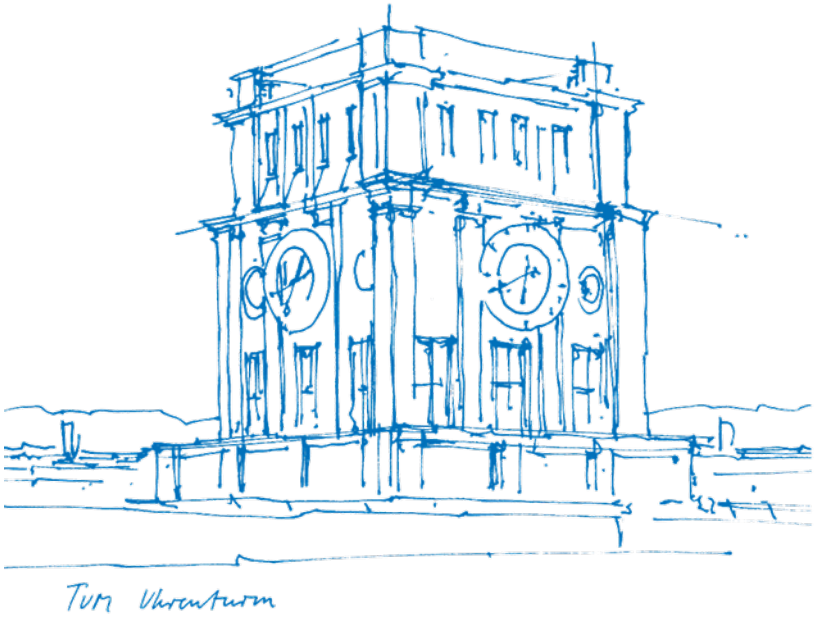
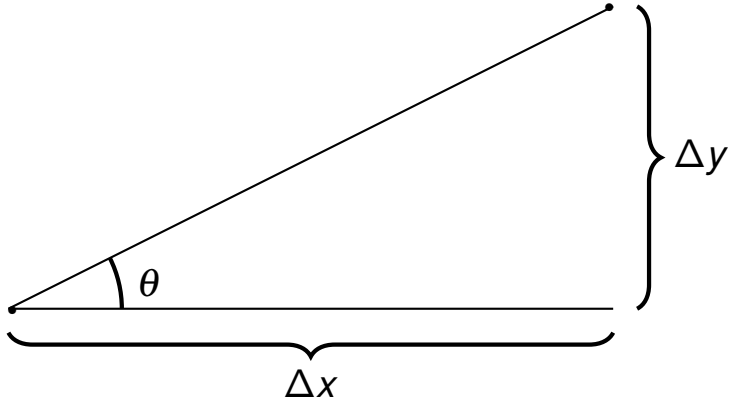
3. November 2022



# 2 Dimensional Force Calculation




$$\Delta x = x_2 - x_1 \tag{1}$$

$$\Delta y = y_2 - y_1 \tag{2}$$

$$|F| = \frac{m_1 m_2}{\Delta x^2 + \Delta y^2} \tag{3}$$

$$F_x = \cos(\theta) \cdot |F| = \Delta x \cdot \frac{m_1 m_2}{(\Delta x^2 + \Delta y^2)^{3/2}} \tag{4}$$

$$F_y = \sin(\theta) \cdot |F| = \Delta y \cdot \frac{m_1 m_2}{(\Delta x^2 + \Delta y^2)^{3/2}} \tag{5}$$

# Utilizing $F_{ij} = -F_{ji}$

The naive approach ($n \cdot (n-1)$ Force calculations):

```
for all Particles p:
        for all Particles p'!=p:
                computeF(p,p')
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A better approach ($\frac{1}{2}n \cdot (n-1)$ Force calculations):

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for all ParticlePairs (p,p'):
        computeF(p,p')
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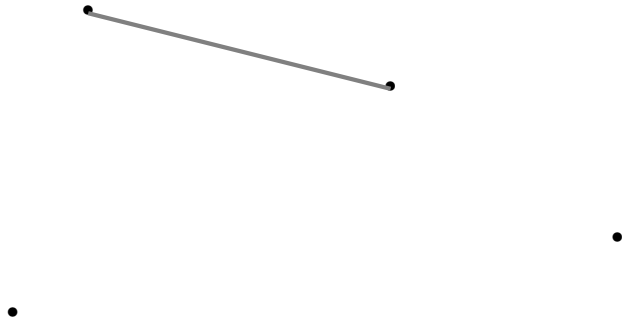

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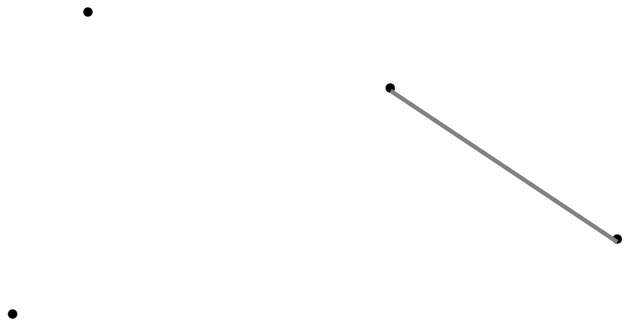

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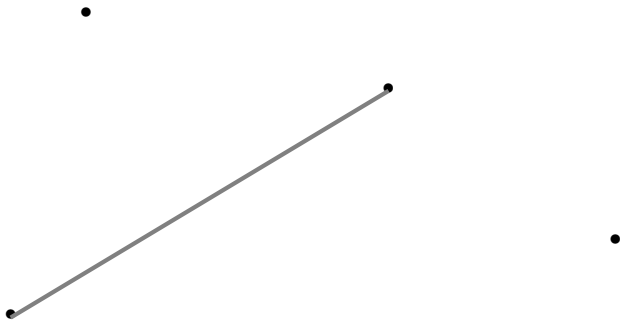

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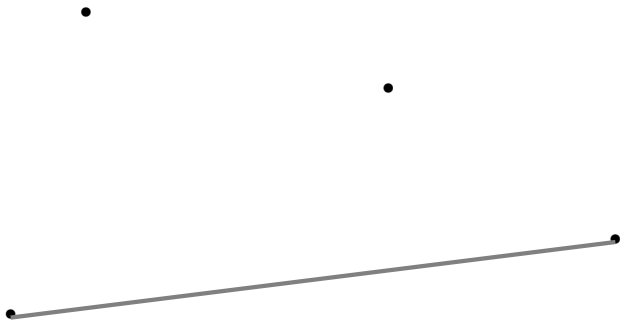
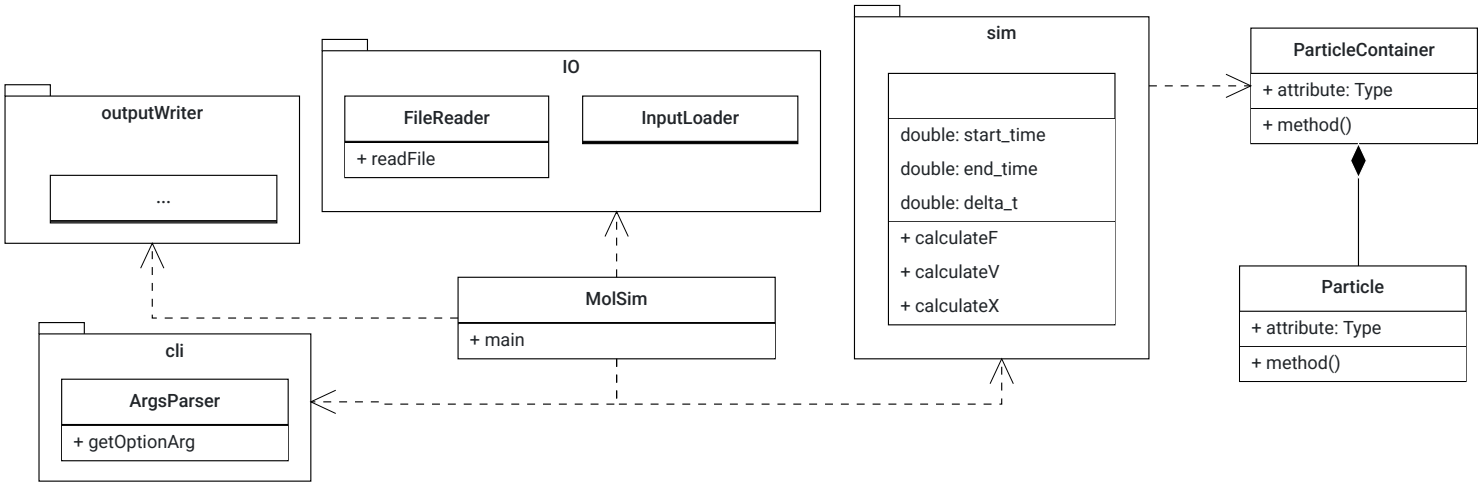


# Refactoring



# Use of the Program

```
 ./MolSim --help
Welcome to MolSim Help
Usage:
MolSim <input-files> <options>
Options:
--help, -h              Prints this screen.
-dt <value>             Sets delta time to <value>. If -dt is not specified default value is used.
-et <value>             Set end time to <value>. If -et is not specified default value is used.
-o <name>               Set base name of output files. DO NOT USE A PATH! Default is 'result'.
-of <path>              Set path to output folder. Default is ./output
```

# Generic IO

```
template <typename LOCATOR, void (*LOAD)(LOCATOR, std::list<Particle>&)>
class InputLoader {
        private:
        std::list<Particle> buffer;
        LOCATOR locator;
        public:
        explicit InputLoader(LOCATOR loc) : locator(loc) {}
        InputLoader(const InputLoader& i) = delete;
        void reload() { LOAD(locator, buffer); }
        void getParticles(std::vector<Particle>&buf) {...}
};
```

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- floating point operations are not associative $\rightarrow$ both outputs were „correct“
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- Funfact: Compiling the exact same code with the exact same compiler settings will result in the same output
- First-hand encounter of the inaccuracies of numerical programming

# bloopers

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- Cmake, Doctest details
- Iterator-related debate
- Data structure locality (for later exercises)