# Molecular Dynamics - Assignment 2

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# Example of new input file

```
#Random comments
# xyz-coord     velocity        mass        shape      dimensions     distance
2
0.0 0.0 0.0     0.0 0.0 0.0     1.0
7.0 7.0 7.0     1.0 1.0 1.0     2.0e-8      CuboiD     4       5       6       3.0
# epsilon    sigma
0.1         0.2
```

Structure:
- Comments
- Number of bodies

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- Bodies (with Shape, Dimensions and distance as optional)

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Structure:
- Comments
- Number of bodies
- Bodies (with Shape, Dimensions and distance as optional)
- Comments
- Definition of epsilon and sigma (optional)

# CI/CD

- Protection of master branch

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- Deployment of CI/CD pipeline for *all* branches

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- library installment

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- sanitizers

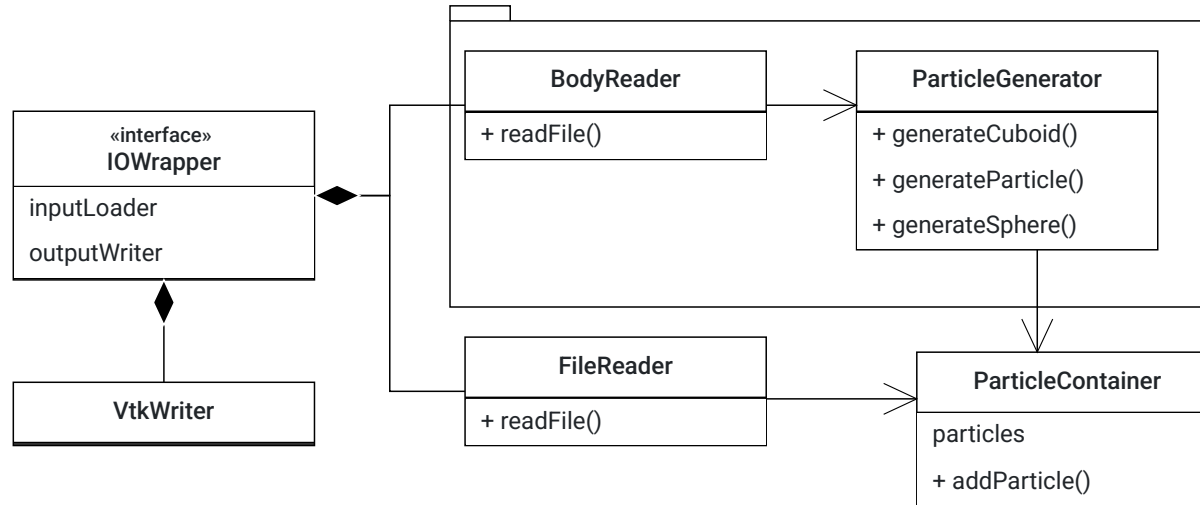# CI/CD

- Protection of master branch
- Deployment of CI/CD pipeline for *all* branches

The pipeline consist of:

- library installment
- build process
- sanitizers
- custom tests

input Loader gets chosen at compile time

# Input parsing - Definition of Body

```cpp
enum Shape {cuboid, sphere};

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

# Performance optimization

Force calculation is the only part relevant to performance

```cpp
void calculateFLennardJones() {
    //set all current forces on all particles to 0
    particleContainer.forAllParticles([](Particle &p) {
            p.setOldF(p.getF());
            p.setF({0., 0., 0.});
    });

    particleContainer.forAllPairs([](Particle &p1, Particle &p2){
            calculate force

            p1.add_to_F(force);
            p2.add_to_F(-force);
    });
}
```

# Roadblocker

Spontaneously imploding Laptops and the lessons they teach us

- Get yourself familiar with alternative options available to not completely disrupt your workflow

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Other Roadblocker

- Missing overview over the already existing functionality and helper functions