Scientific Computing (PSE) Molecular Dynamics
Group D

Worksheet 2

02

PROJECT TASKS

Task 1 to 3 -Worksheet 2

Unit Testing

Integrated testing in CMake using the googletest suite

Continous Integration

CI tools provided by GitHub

Logging

adding meaningful log messages in runtime using spdlog

Testing and CI

googletest integration for previous methods

Restructuring and Logging

to make the project ready for new functionality

New implementation

File parser, Lennard-Jones forces and simulation

TIMELINE

We used most of the time for refactoring, restructuring, testing, logging and performance improvements so that the simulation task itself was fairly easy to implement and quickly done

04

COLLISION SIMULATION TASK

Task 4

Particle generator

particle generator that can initialize the simulation

Lennard-Jones forces

The interaction between two molecules i and j

Simulation

perform 2D simulation of the collision with the given parameters

EXPECT_

```
EXPECT_TRUE(cond1)
    EXPECT_EQ(val1, val2)
        EXPECT_NE(val1, val2)
            EXPECT_DOUBLE_EQ(val1, val2)
```

vs.

ASSERT_

```
ASSERT_FALSE(cond1)
    ASSERT_GE(val1, val2)
        ASSERT_FLOAT_EQ(val1, val2)
            ASSERT_ANY_THROW(statement)
```

GOOGLETEST

Advantages

easy to use unit testing with CMake integration

import via FetchContent

Key features

ready-to-use framework, easy setup, automatic executing with ctest

asserts() and expects()

Gravitational force testing

L2-norm = $\sqrt{(x^2 + y^2 + z^2)}$ = Euclidean norm

Multiplied mass of particles = mass1 * mass2 = 1005.34

L2-norm)^3

compute actual forces (by hand)

```
EXPECT_TRUE(calculated_force[0] - actual_force[0] < 0.0000001)

EXPECT_EQ(calculated_force, zero_force)
```

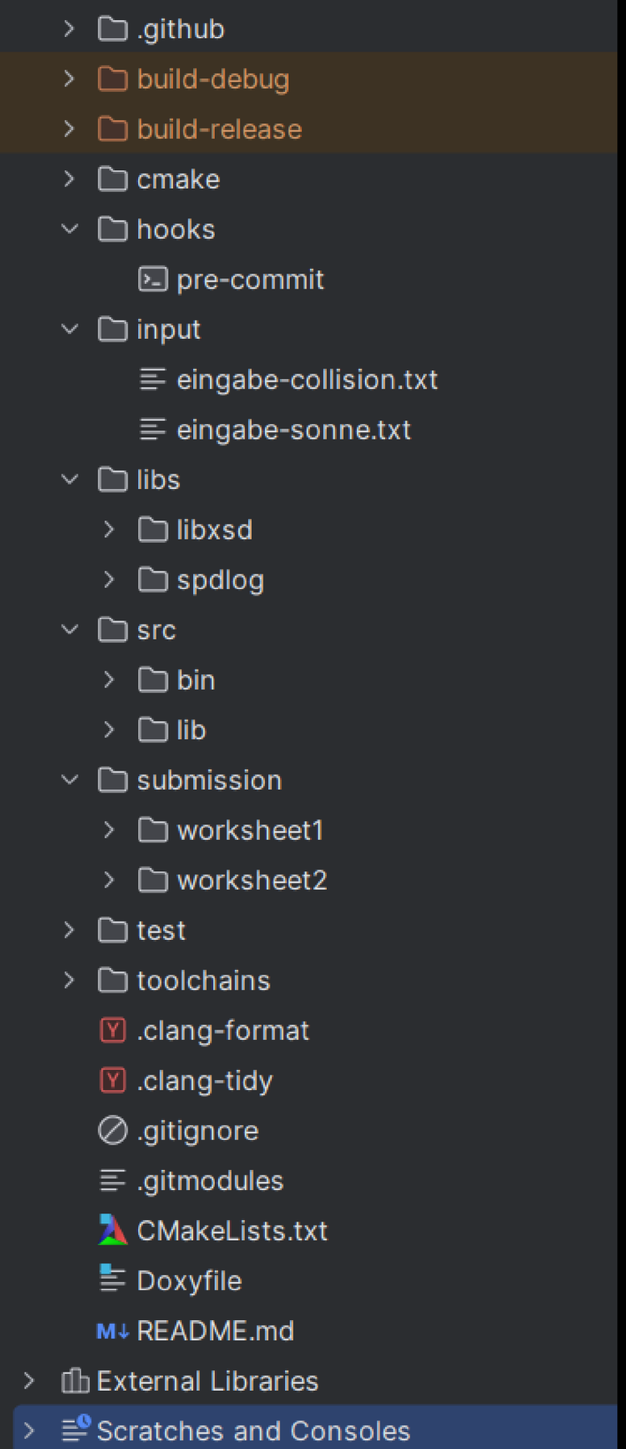
Lennard-Jones force testing

compute displacement of vectors r_ij = || x_i -x_j ||
manually compute the Lennard-Jones potential by hand using the formula
manually compute the Lennard-Jones forces using the formula

```
EXPECT_DOUBLE_EQ(calculated_force[0], actual_force[0])

EXPECT_TRUE(calculated_force[0] - actual_force[0] < 0.0000001)

EXPECT_TRUE(std::isnan(force))
```



REFACTORING

Structure

strongly adjusted the project structure to fit our needs and make the project easier to manage and extend in the coming weeks

split CMakeLists into several files with each one only configuring a specific part like testing, logging, etc. with one high-level list

Naming

snake_case style naming for variables, functions etc.

Log Functions

```
spdlog::info("Message");
```

vs.

Log Macros

```
SPDLOG_INFO("Message")
```

LOGGING

Advantages

Fast, header-only logging library for C++

Key features

Performance, ease of use, flexibility

In use

```
switch (model) {
  case physics::ForceModel::LennardJones: {
    spdlog::info( msg: "Processing Lennard-Jones model.");
    auto cuboids : vector<...>  = *parse_cuboids( &: input_buf);
    spdlog::debug( fmt: "Parsed {} cuboids.", cuboids.size());
    auto p : vector<Particle>  = generate_cuboids(cuboids, config->seed);
    spdlog::debug( fmt: "Generated {} particles for Lennard-Jones model.", p.size());
    particles = ParticleContainer( &: p);
    break;
  }
```

For performance tracing / timings

SPDLOG_LEVEL=ON

SPDLOG_LEVEL=OFF

LOGGING

Advantages

Fast, header-only logging library for C++

Key features

Performance, ease of use, flexibility

MolSim Usage

via command line

```
--output       -o    specify output file
--input        -i    specify input file
--help         -h    open usage page
--delta_t      -d    set delta_t
--start_time   -s    set start_time
--seed         -r    set seed for rng
--end_time     -e    set end_time
--io_interval -l     set plot interval, 0
disables plotting
```

Running simulations...

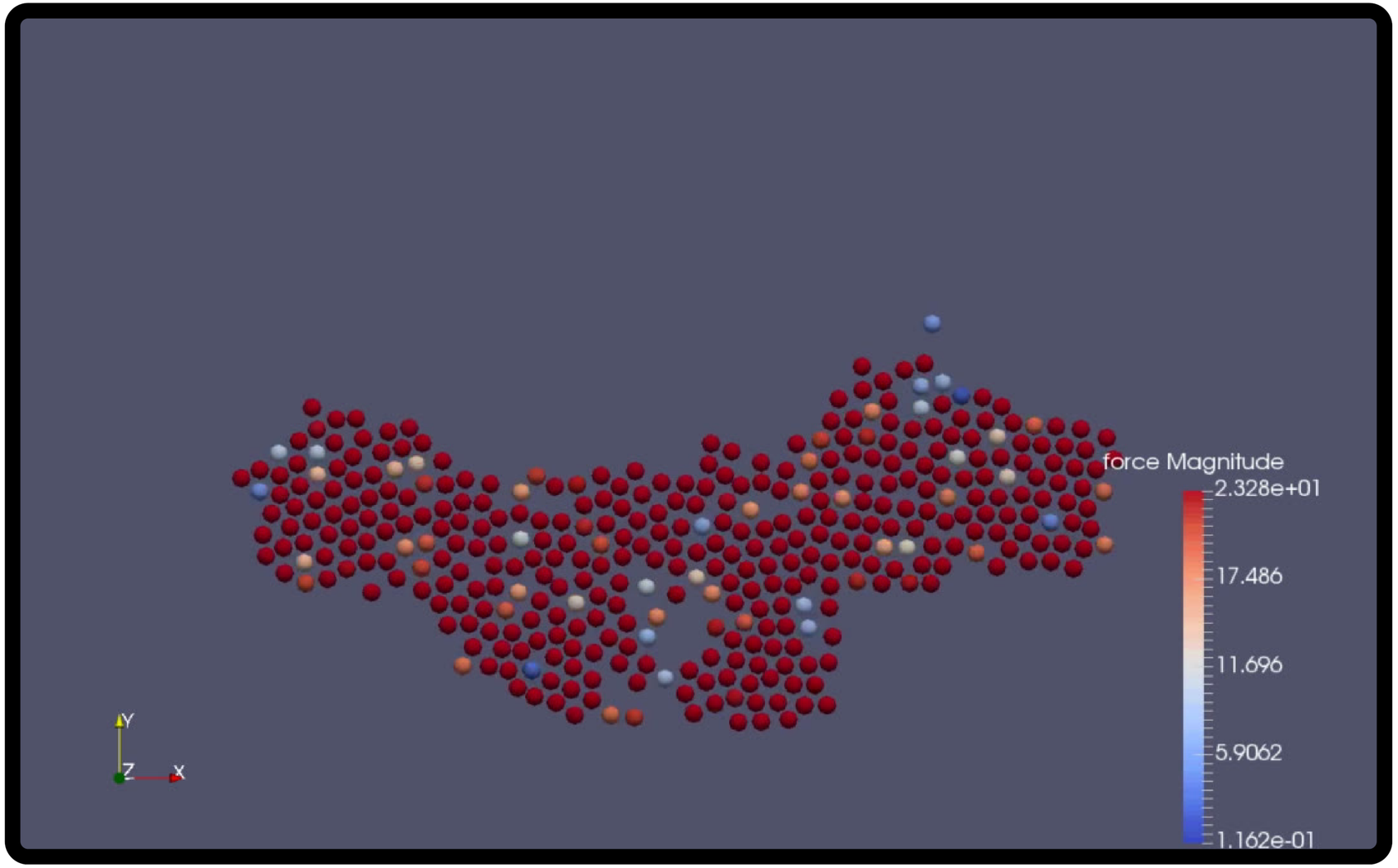
for simulation on worksheet

```
Call: ./MolSim
-o LennardJones
-i “../input/eingabe-collision.txt”
-d 0.0002
-e 5
```

SIMULATION 1

Force magnitude as color code

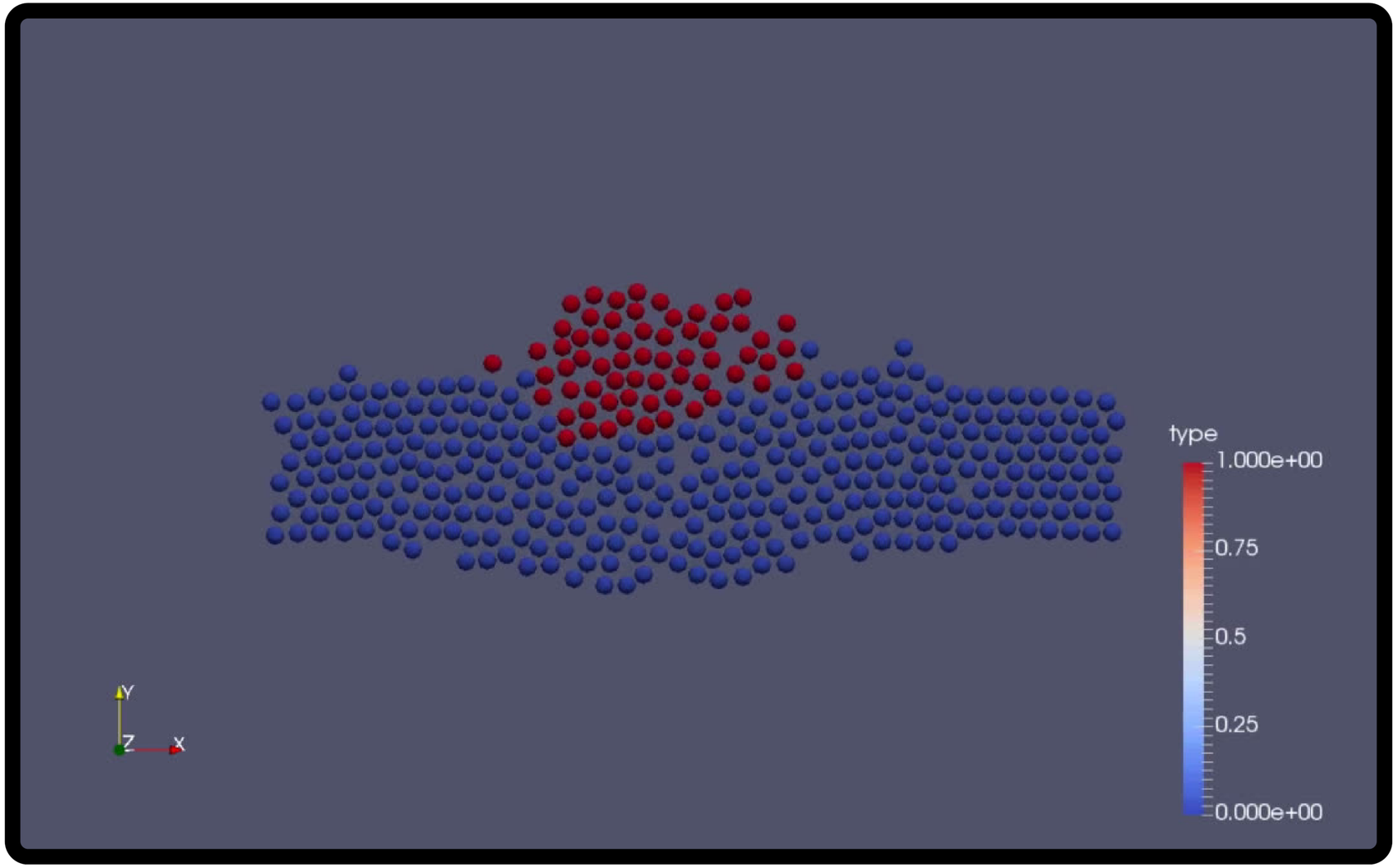
12



SIMULATION 2

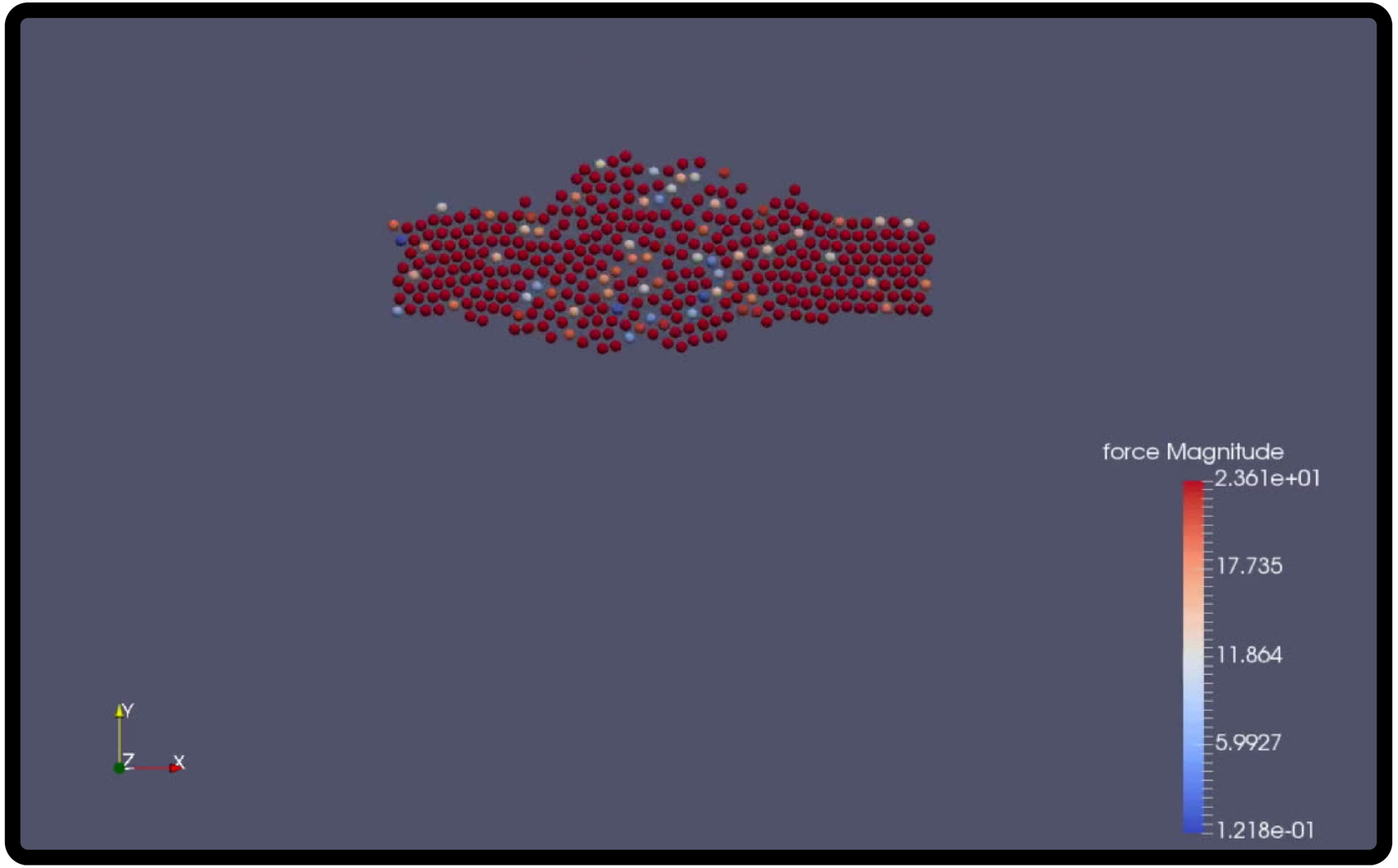
Molecule type as color code

13



SIMULATION 3

Force magnitude as color code



SIMULATION TIMES

on our different setups

Function Call

./MolSim
-o LennardJones
-i “../input/eingabe-collision.txt”
-d 0.0002
-e 5

01:23:652 min

Hardware: AMD Ryzen 9 7950X3D 16C/32T, 64GB RAM
WSL on Windows 11

01:24:964 min

Hardware: Intel i5-12600K 10K/16T, 32GB RAM
WSL on Windows 11

01:33:020 min

Hardware: Intel i7-8750H 6C/12T, 32GiB
Linux only system

SUMMARY & LEARNINGS

TASK 1

testing for correct behavior with pre-calculated result checking
testing is important and helpful and can save a lot of time (and also take a lot of time...)

TASK 2

checking for correct formats, running tests, checking code quality with clang-tidy, sanitizers
leads to clean repository and prevents bad/non-functioning code from being merged into the main branch

TASK 3

cleaner faster and uniform possibility to print to terminal, way better than printing out single values and steps

REFACTORING

meaningful naming, tidy structure, saves lots of time and makes working in a group more efficient

FUTURE IMPROVEMENTS

PERFORMANCE

parallelization, use of multi-core and threading
streamline calculation
switch logging to macros for better runtime performance which did not work properly for us at this point

TESTING

more edge case tests
writing tests while implementing new methods

ADJUST PARSER

we thought about implementing an XML parser already but did not yet
will be necessary for next week’s worksheet

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THANK YOU FOR LISTENING