Worksheet 1

Scientific Computing PSE Molekulardynamik

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About First Steps

- One full Linux/Ubuntu user
- Two Windows users with Windows Subsystem for Linux (WSL)
- JetBrains Clion as IDE

- visualization tools from the student starter clues
- branching for different features

- Task 2 and initial pull request in GitHub as specified in worksheet

Task 3

- Followed instructions of the worksheet
- Calculations of position, force and velocity according to the formulas in the slides

- optimized performance by calculating forces in pairs as computation is only necessary once

Task 4

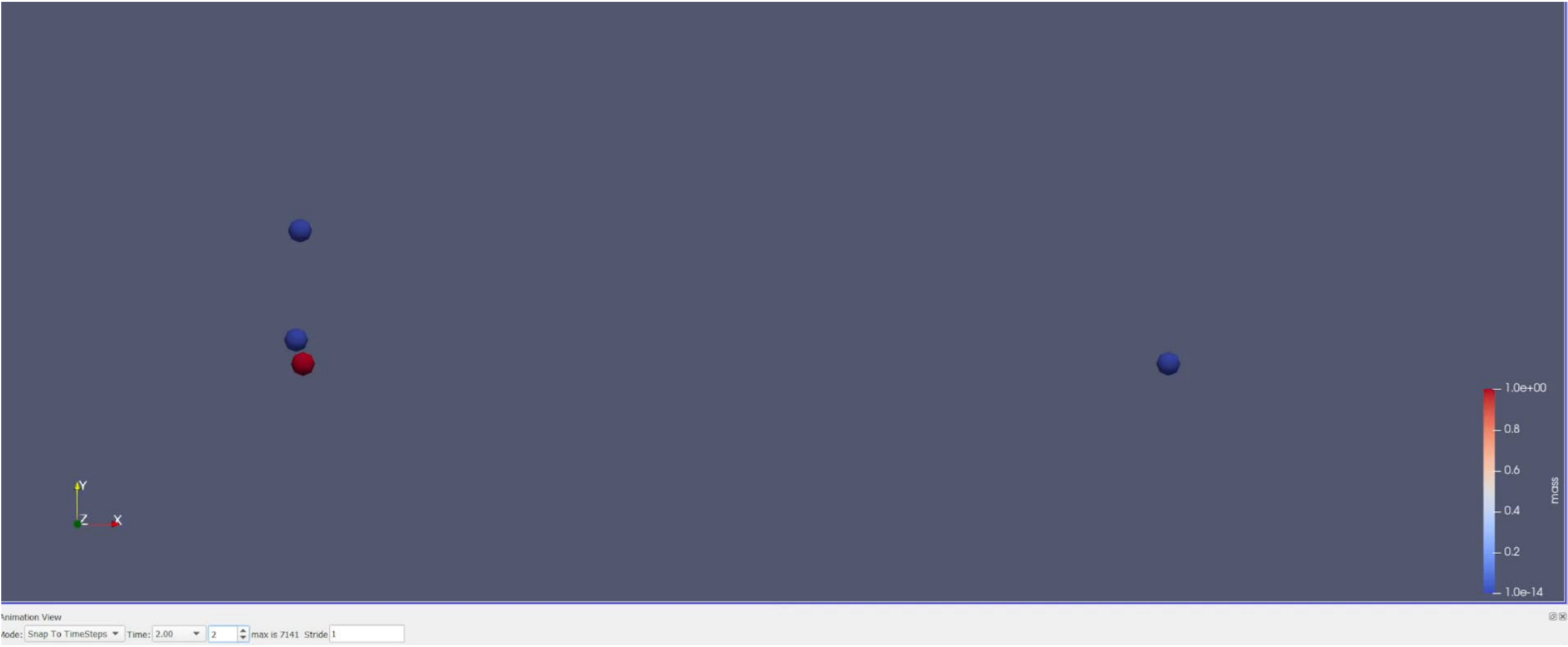
- Simulated and visualized in ParaView with the given values of delta_t and t_end

- Decision about celestial bodies based on the given masses in eingabe-sonne.txt and their trajectories in the simulation

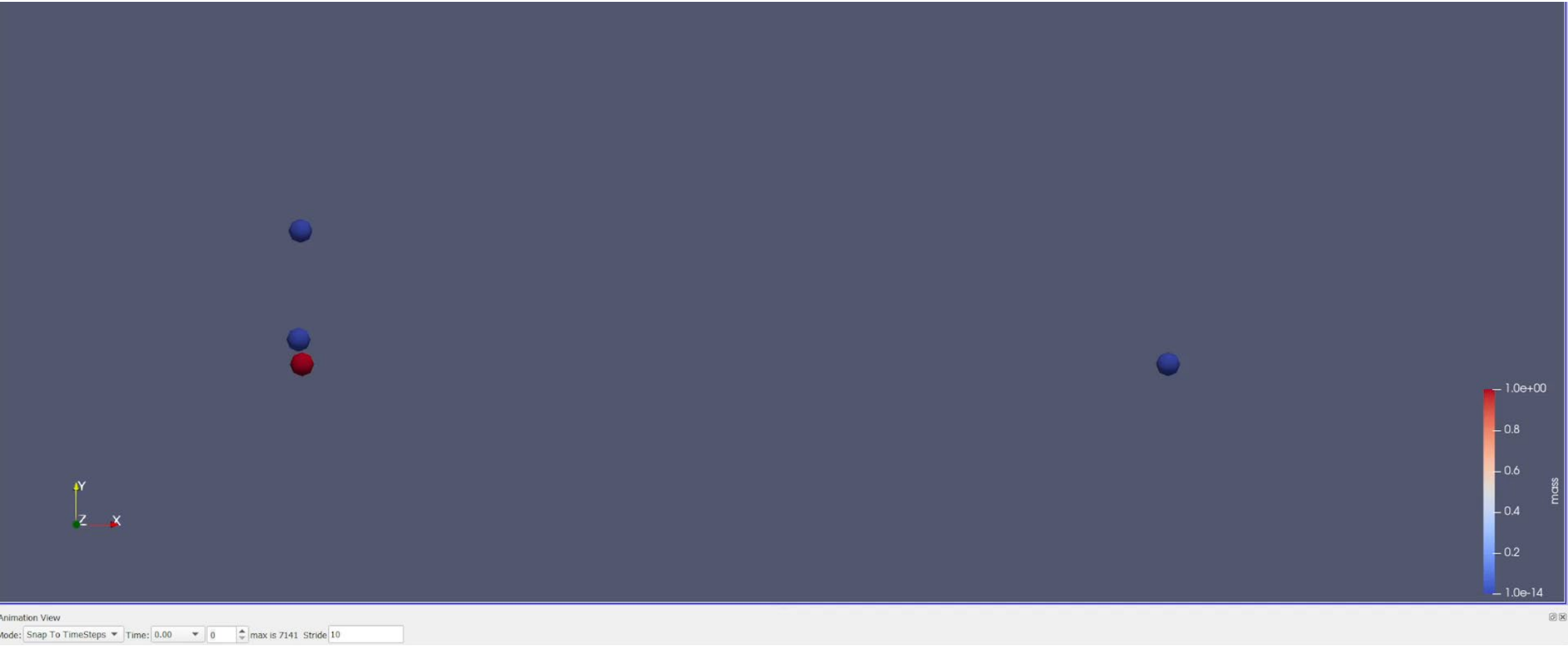
Celestial bodies in ParaView

Celestial bodies with forces in ParaView

Animation Stride Size 1



Animation Stride Size 10



Animation Stride Size 40

Task 5

- Encapsulation of particles in the class ParticleContainer

- Iterator pattern seemed like a reasonable choice to us
- Strategy pattern could be used for abstraction of different force calculations

- Switched to using a vector to store particles for now

Task 5

- Added doxygen as documentation tool and adjusted the configuration options
- Annotations and comments in new code implementations for doxygen to use
- Checked doxygen output as html and LaTex/pdf