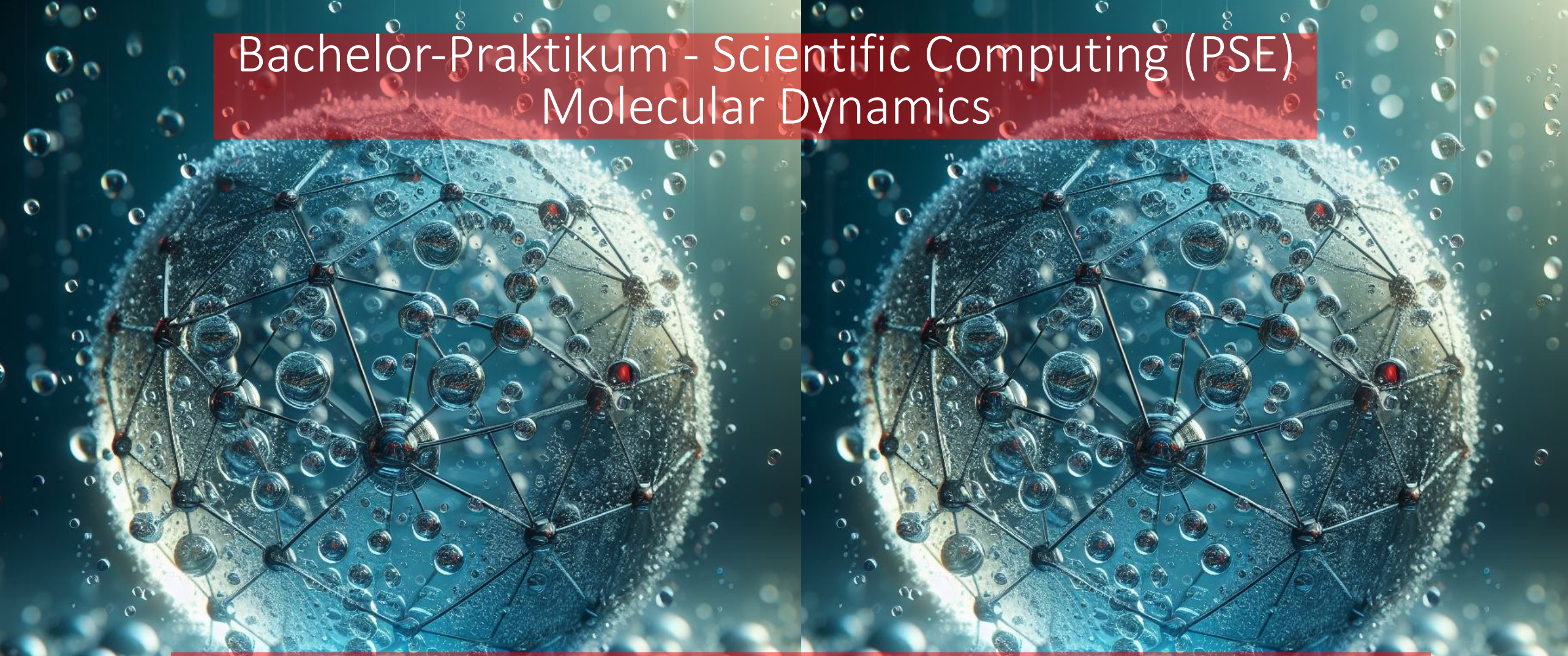
Bachelor-Praktikum - Scientific Computing (PSE)
Molecular Dynamics



- Worksheet 3 – Linked Cell Algorithm and the Falling Drop

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Input Format

- We ❤️ JSON: sweet spot between human- and machine-readability

```
"objects": [
  {
    "type": "cuboid",
    "type_id": 1,
    "position": [2, 9, 1],
    "velocity": [-15, 0, 0],
    "size": [5, 5, 1],
    "mesh_width": 1.1225,
    "mass": 1
  },
  {
    "type": "cuboid",
    "type_id": 2,
    "position": [13, 9, 1],
    "velocity": [15, 0, 0],
    "size": [5, 5, 1],
    "mesh_width": 1.1225,
    "mass": 1
  }
]
```

```
"simulation": {
  "model": "lennard_jones",
  "particle_container": {
    "type": "linked_cell",
    "dimensions": [20, 20, 3],
    "cutoff_radius": 3,
    "boundary": {
      "all": "reflective",
      "right" : "outflow"
    }
  },
  "end_time": 2,
  "time_delta": 0.0002,
  "video_duration": 30,
  "frame_rate": 24,
  "output_type": "vtk",
  "output_path": "output",
  "sigma": 1,
  "epsilon": 5
},
```

Inspired by CSS: more specific modifiers override more general ones. In this case, all boundaries except ‘right’ are reflective. The boundary on the right is set to ‘outflow’.

Linked-Cell Particle Container

- **Reflective and Periodic Boundaries** on all three axes independently for seamless and realistic particle interactions. Reflects particles based on specified boundary behaviors for each border.

- **Efficient Data Organization** using a 1D vector to store a 3D grid of cells, optimizing memory usage.

- **Reflection Mechanism:** Adjust the position and the velocity of particles by mirroring them.

- **Challenges…**

Things we had to think about

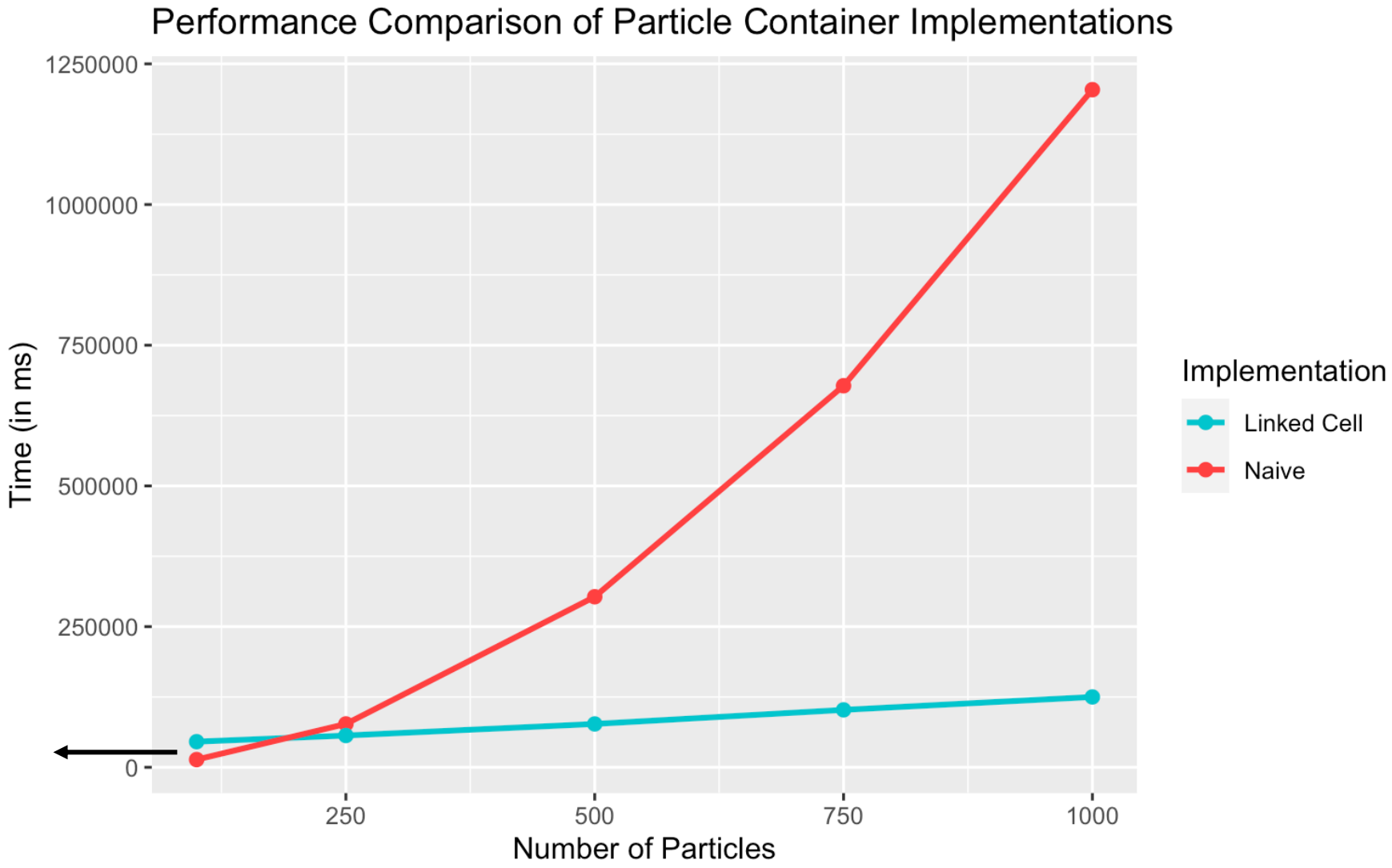
- **3D-1D cell index conversion:** How to address particle cells?
  - Our first solution was particularly segfaulty. We tried to put articles into non-existing cells…
- **Reflective boundaries:** How to reflect particles?
- **Disappearing particles?**
- **What to do about domain size not being multiples of the cutoff radius?**

Impressive Performance Boost

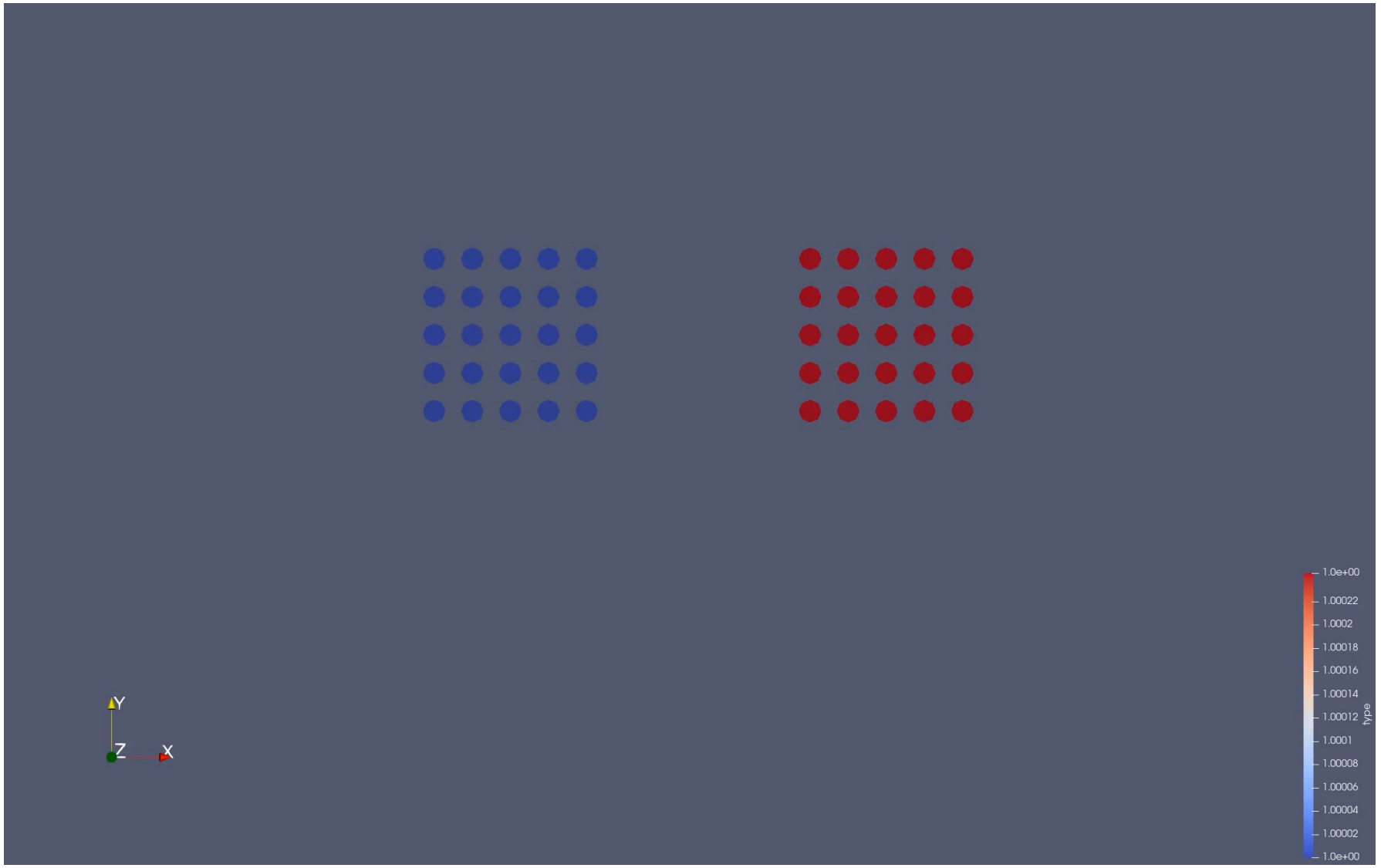
Linked cell:
Needed time grows in a linear fashion

Old implementation:
Exponential growth

With 100 particles, the naïve implementation is faster than the linked cell implementation because of the overhead of managing cells

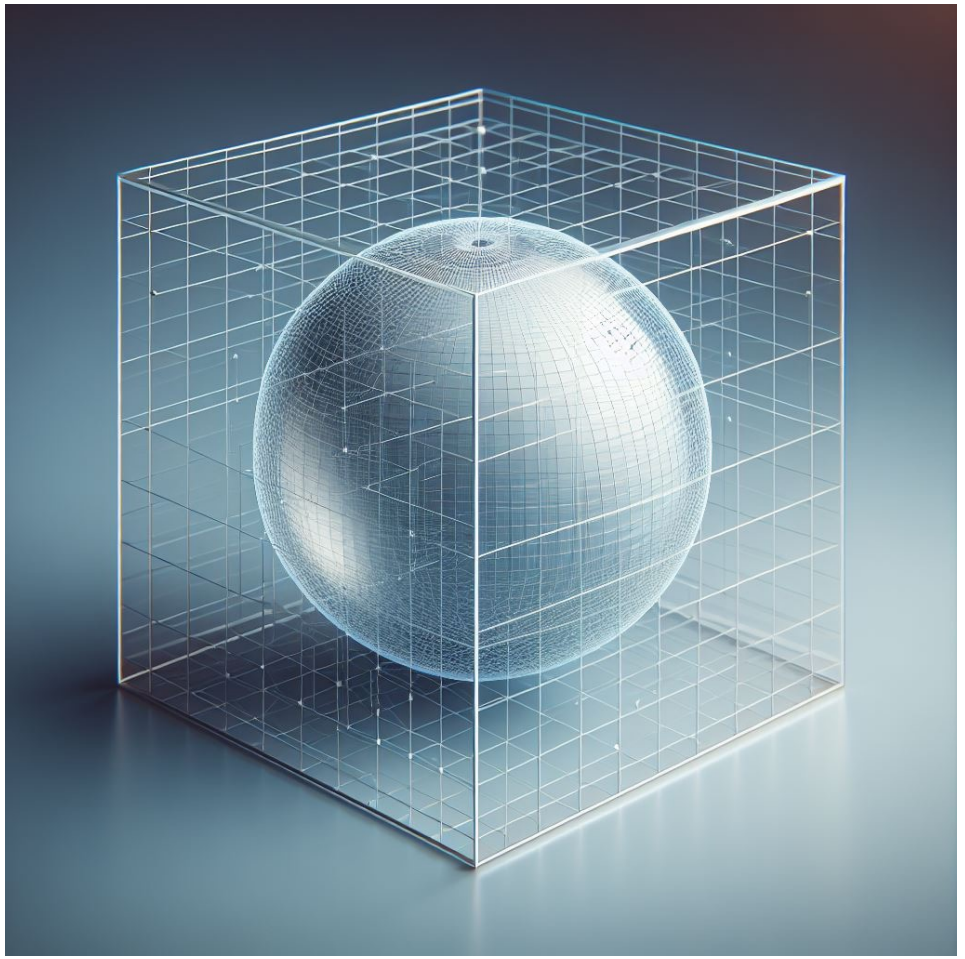


Different Boundary Conditions Visualized



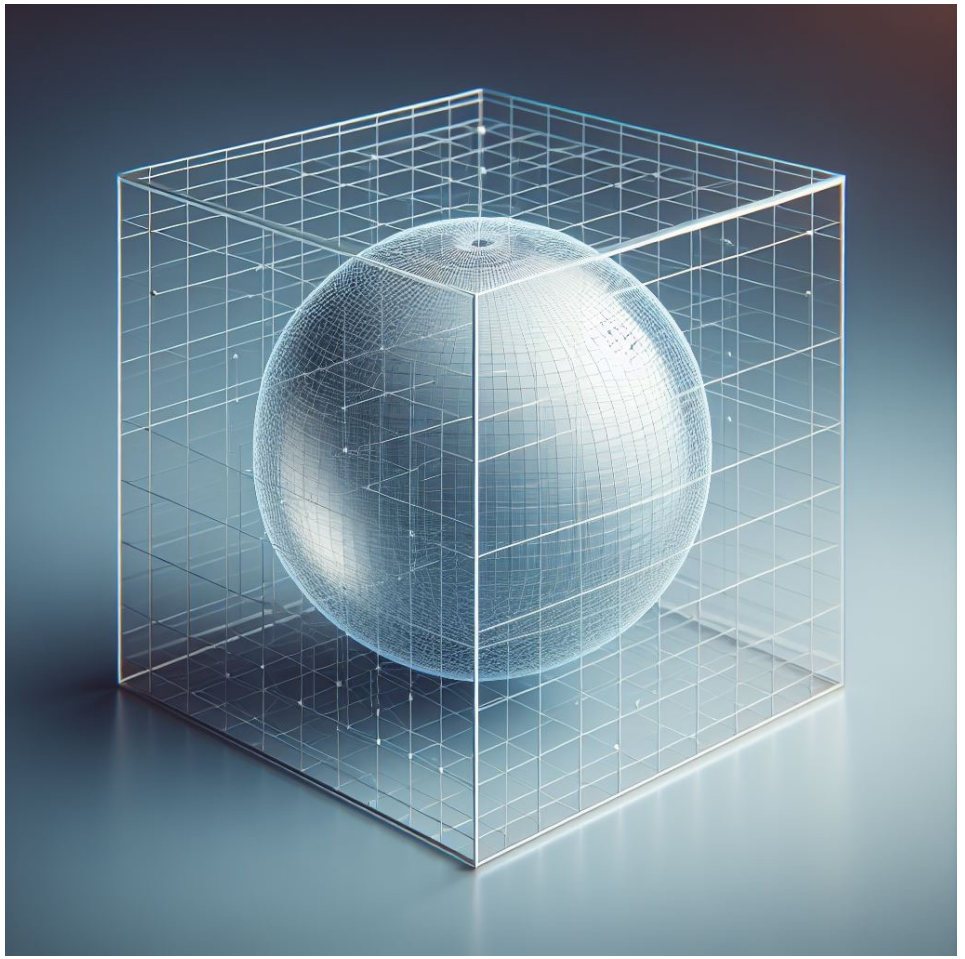
Particle Generator - Sphere

- Generate particles within a cubic region only if they’re within the spherical boundaries
- The Gauss Circle Problem and lattice points in 3D
- Challenge: Testing the exact amount of generated particles

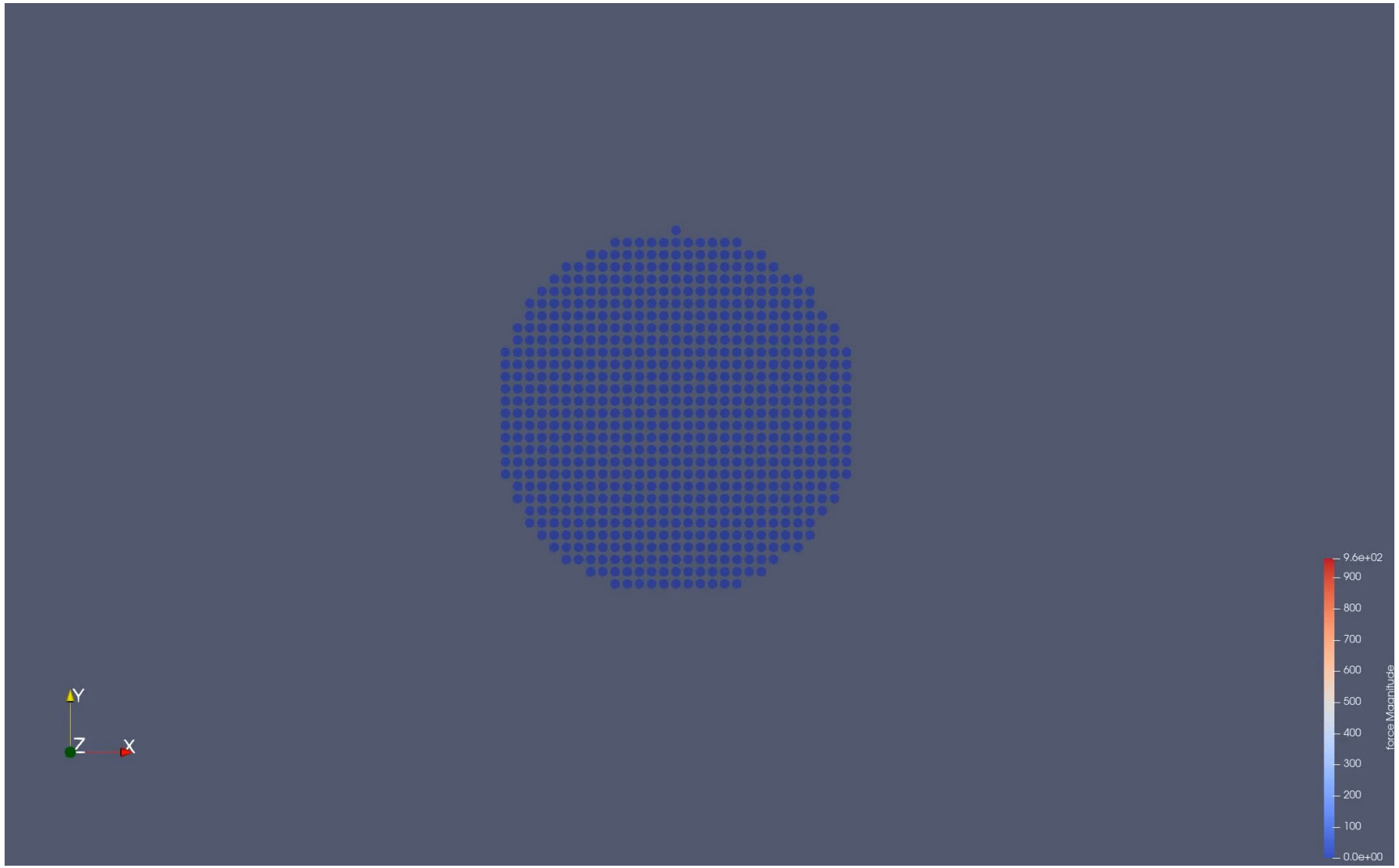


But our animation is 2D

- Implement a disk generator
- Very similar to the sphere generator, only 2D.



Falling Drop - Reflective Boundaries



References

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