MolSim WS 23/24

Sheet 3

XML, Linked-cell algorithm and

“falling drop - Wall”

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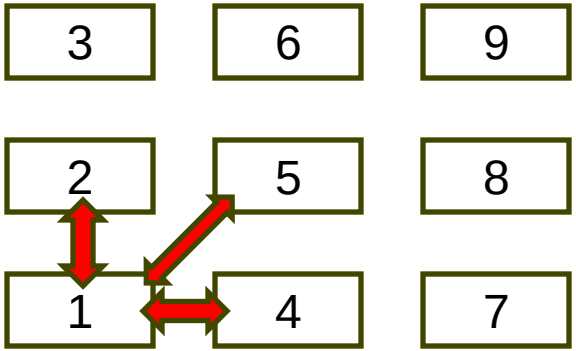
XML- Input

- **Create a xml-schema**
  - ⇒ We oriented ourselves on our own classes
  - ⇒ e.g. element for a particle container
  - ⇒ Less complex code
- **Use of adapter pattern**
  - ⇒ e.g. XSD-Cuboid to Cuboid-Spawner

Linked-Cells-Algorithm

- **Implementation & Optimizations:**
  - Essentially a list of cells
  - Additional data structure for optimization

    ⇒ lists for: occupied-, halo-, neighbor-...cells
  - Utilize Newtons 3rd law on particle and cell level



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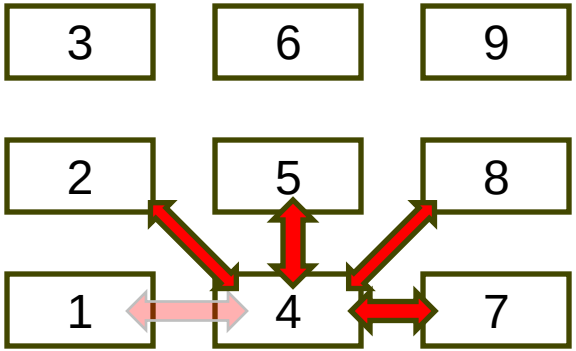
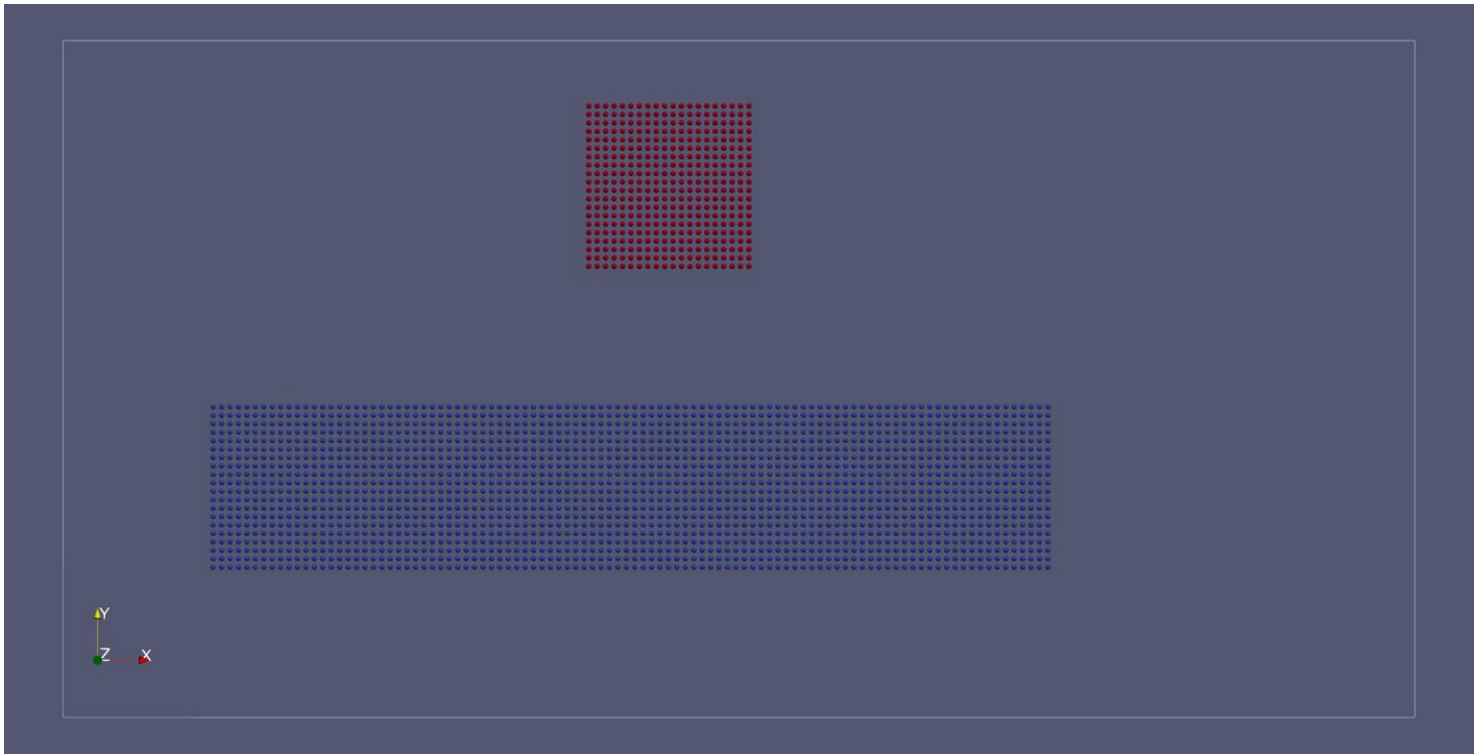


Linked-Cells-Algorithm



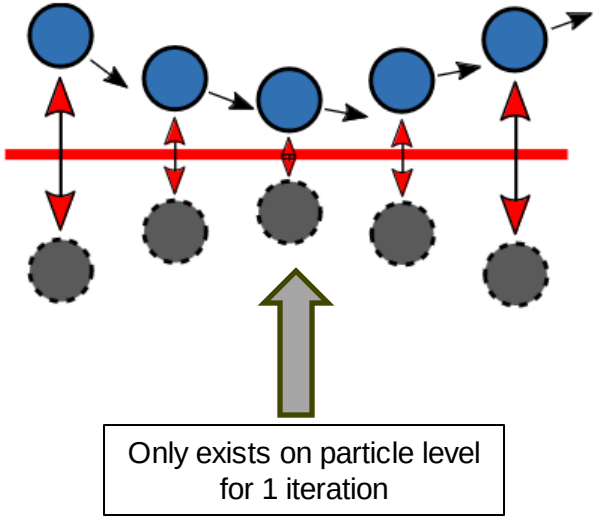
Linked-Cells-Algorithm

- **Outflow Boundaries:**
  - Simple implementation

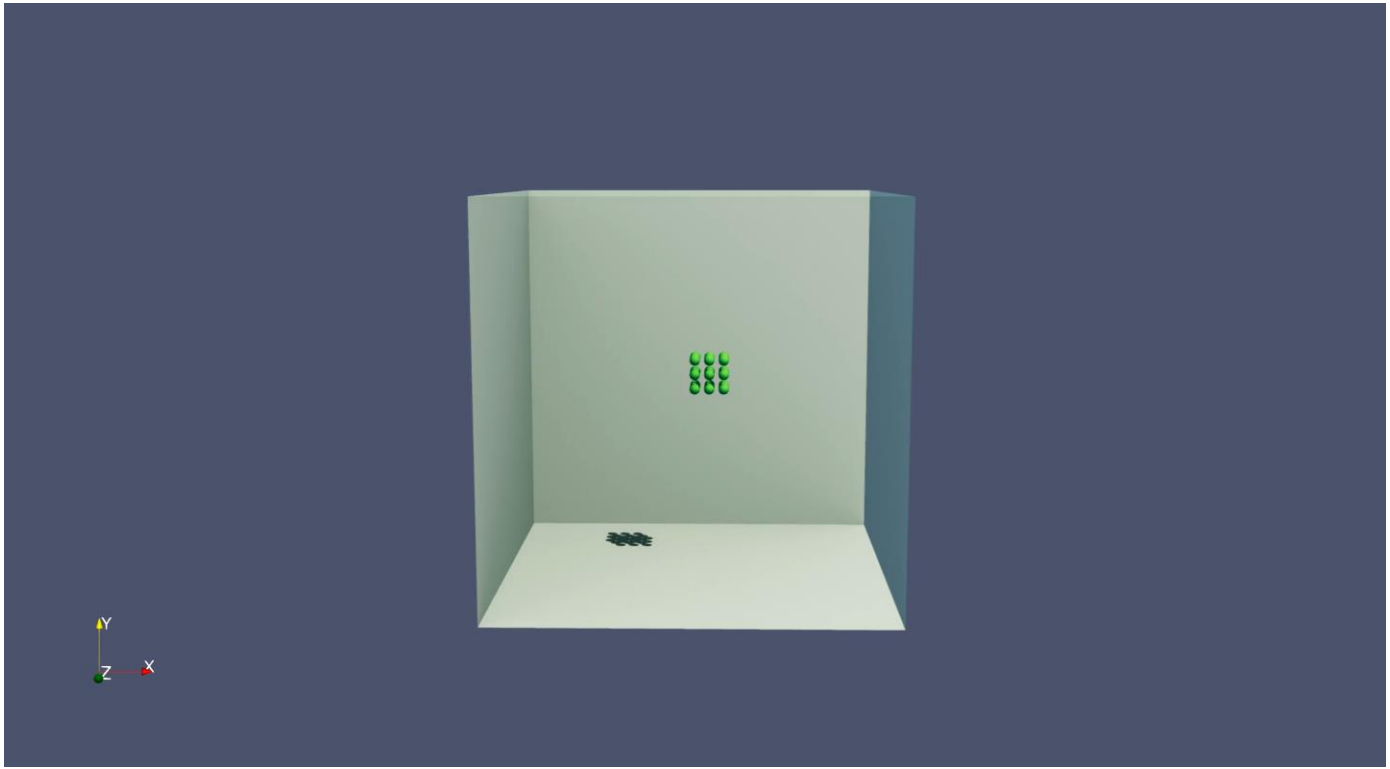
  ⇒ Delete particles in halo cells
- **Reflective Boundaries:**
  - Creation of hypothetical particle
  - We don't save ghost particle

  ⇒ more memory efficient

  ⇒ less complex in our code base



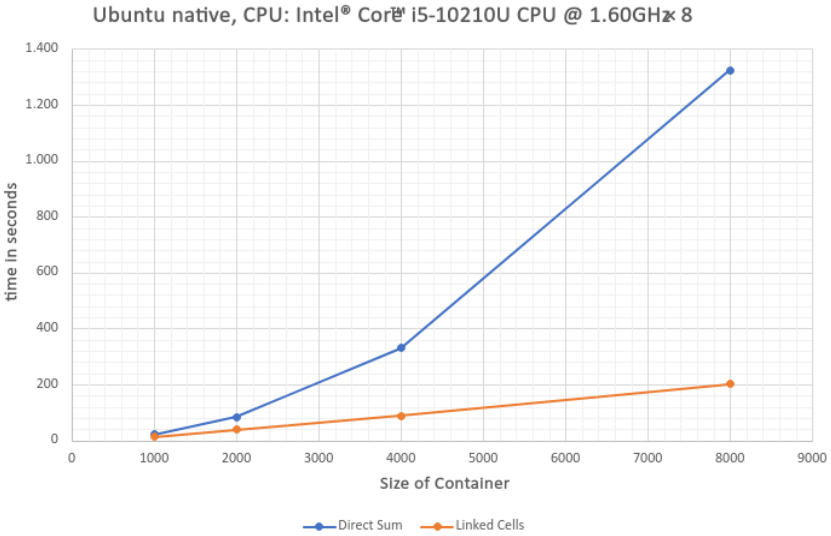
Linked-Cells-Algorithm



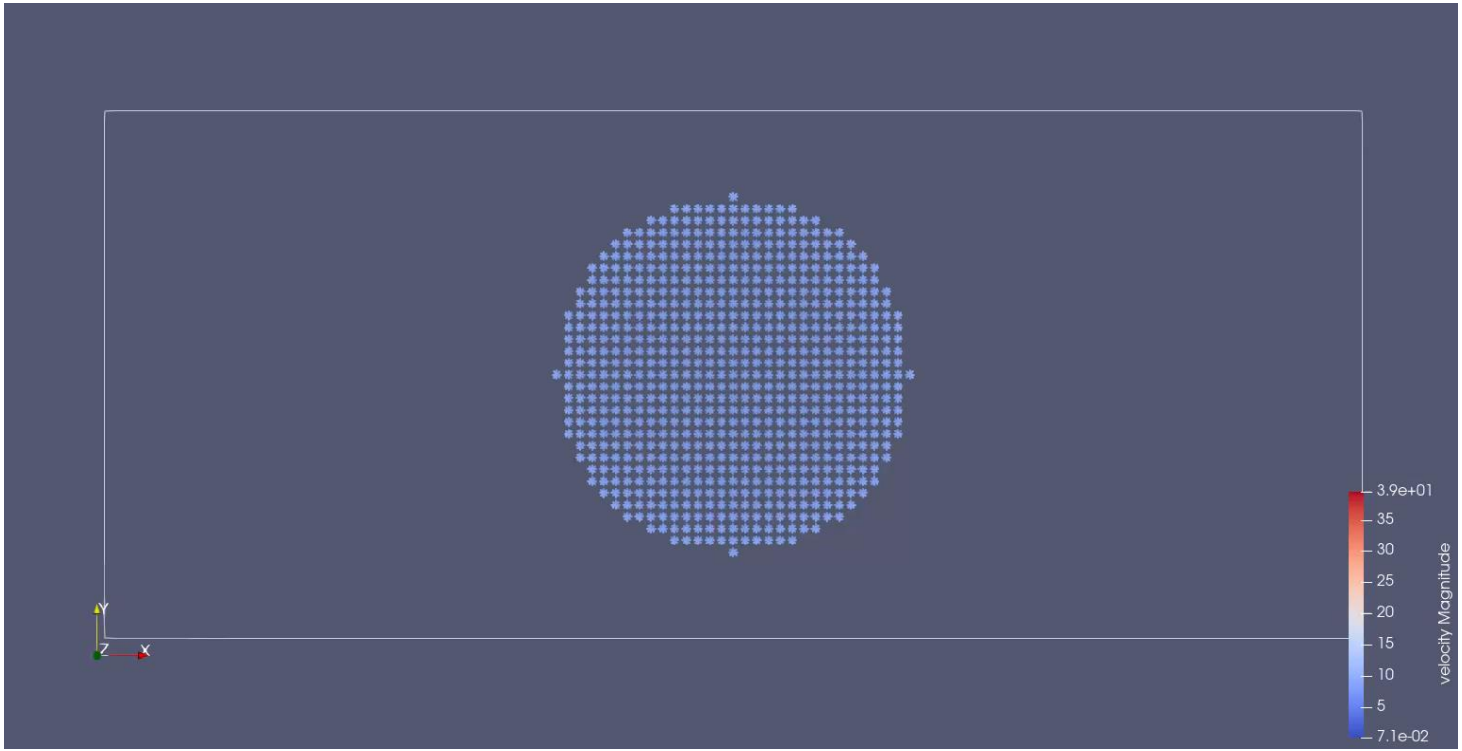
Linked-Cells-Algorithm

- **Performance:**
  - We tested on WSL and native Linux
  - Direct sum container: Quadratic Growth
  - Linked Cells container: Linear Growth

  ⇒ Very good approximation



Simulation of a falling drop - Wall



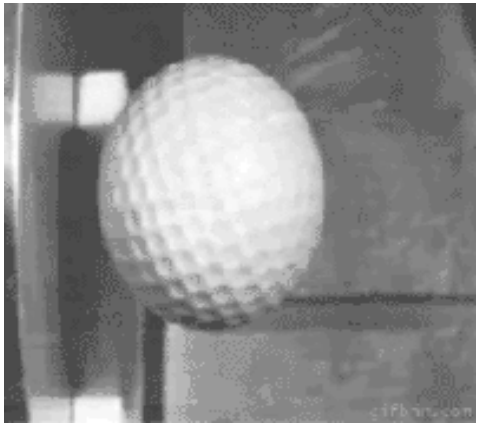
Simulation of a falling drop - Wall

- **Expectations:**
  - Forces only between particles

  ⇒ should look like a water drop in space
- **Observation:**
  - Snowball contracts and then scatters
  - Macro scale(looking at ball as one object):

Kinetic energy ⇒ Deformation energy ⇒ Kinetic energy

  - Deformation becomes an emergent phenomenon



Summary of cool things

- We enabled XML-Input
- We accelerated our simulation with a new container
- We drew a pretty performance plot
- We implemented boundaries and simulated balls bouncing in an aquarium
- We made a pretty video of a snowball thrown at a wall

References

Adapter picture: https://www.amazon.de/Digital-Multiport-Schnellladeanschluss-2016-2022-2018-2022-Wei%C3%9F/dp/B0BPJQYVQ3
Golf ball collision: https://gifer.com/en/gifs/collisions