

# MolSim WS 23/24

Sheet 3

XML, Linked-Cell-Algorithm and

“Falling Drop - Wall”

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05.12.2023

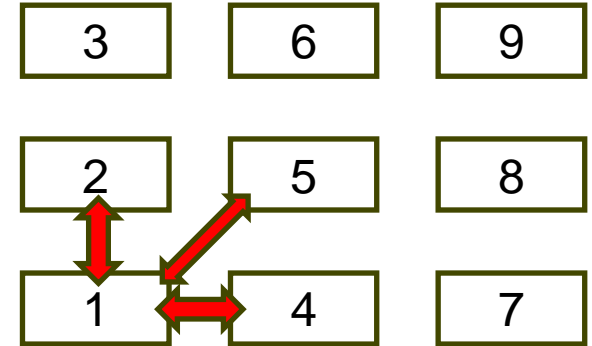
# XML- Input

- **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



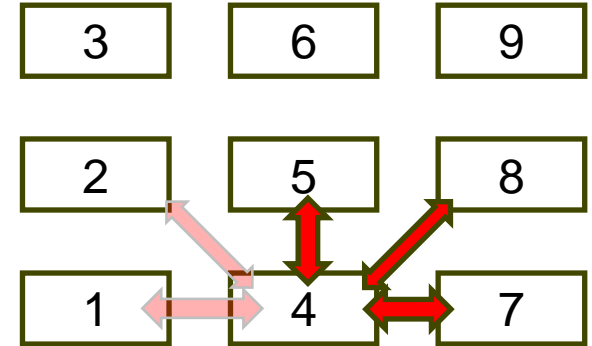
# Linked-Cells-Algorithm

- **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

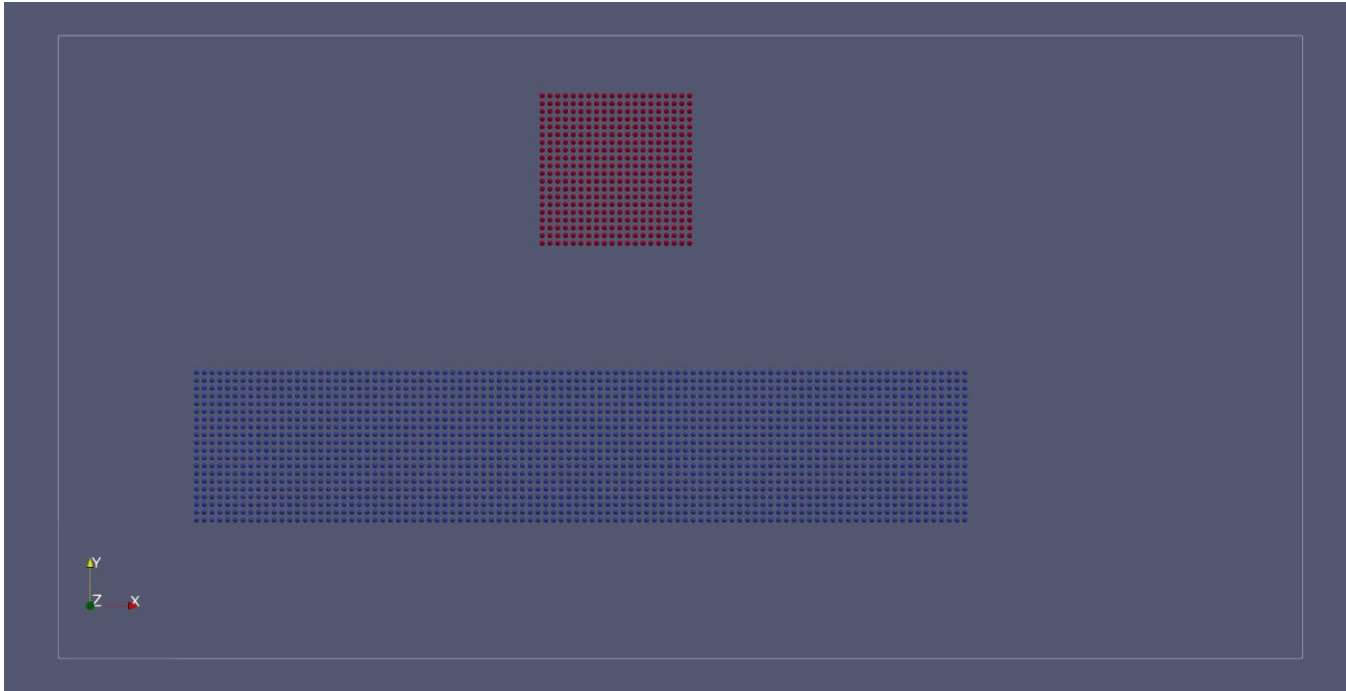


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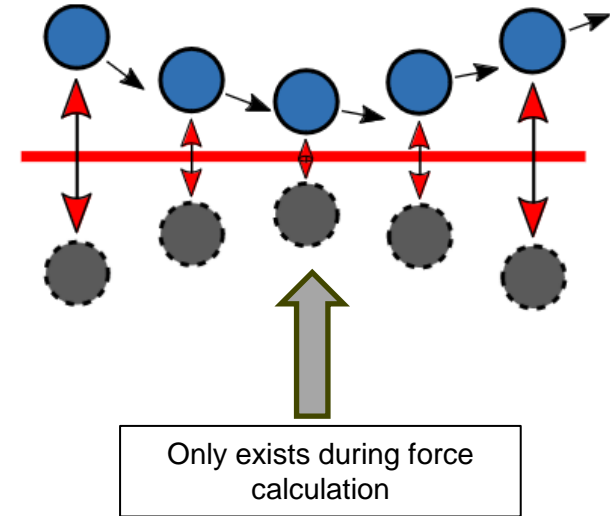
# Linked-Cells-Algorithm



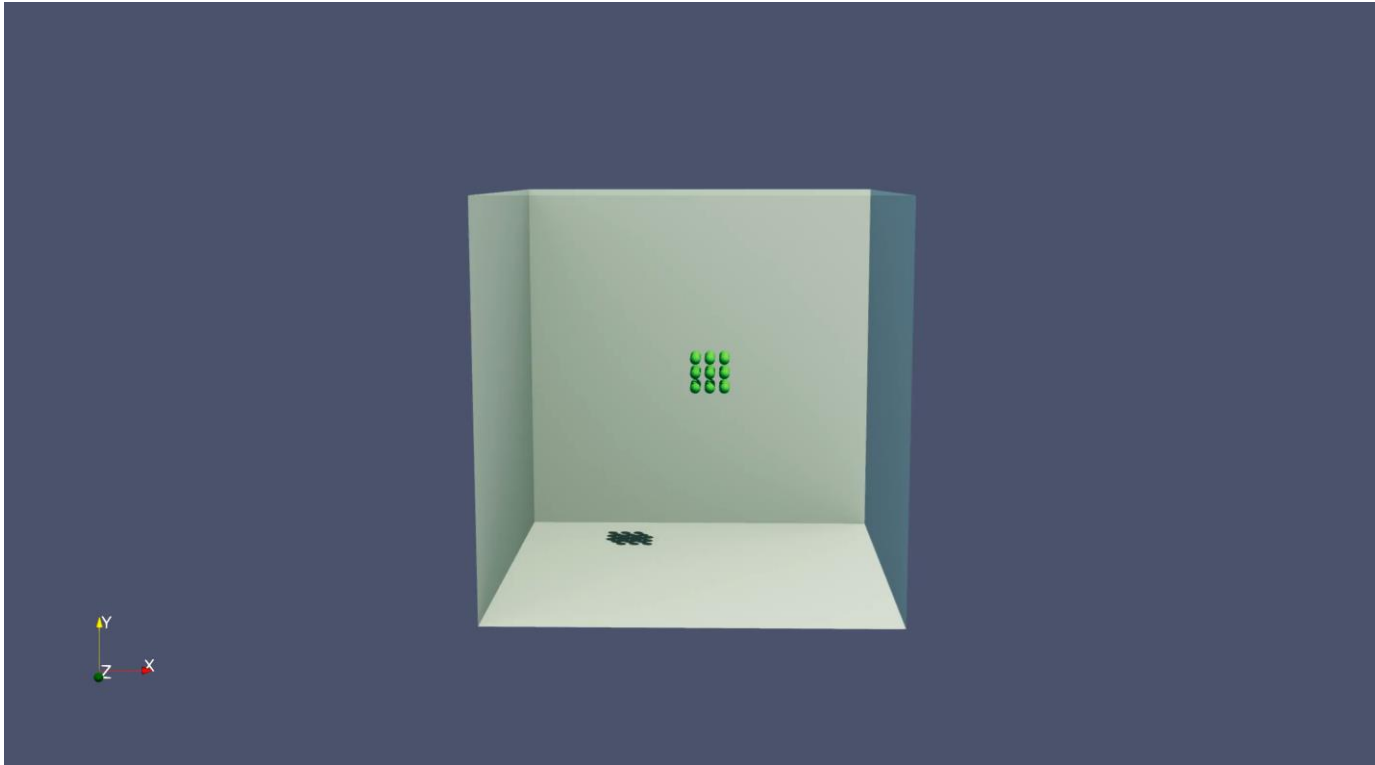
<https://manuellerchner.github.io/MolSim-WS23-24/submissions/>

# Linked-Cells-Algorithm

- **Outflow Boundaries:**
  - Simple implementation
  - ⇒ Delete particles in halo cells
- **Reflective Boundaries:**
  - Creation of hypothetical particle
  - Ghost particle is not saved
  - ⇒ more memory efficient
  - ⇒ less complex in our code base

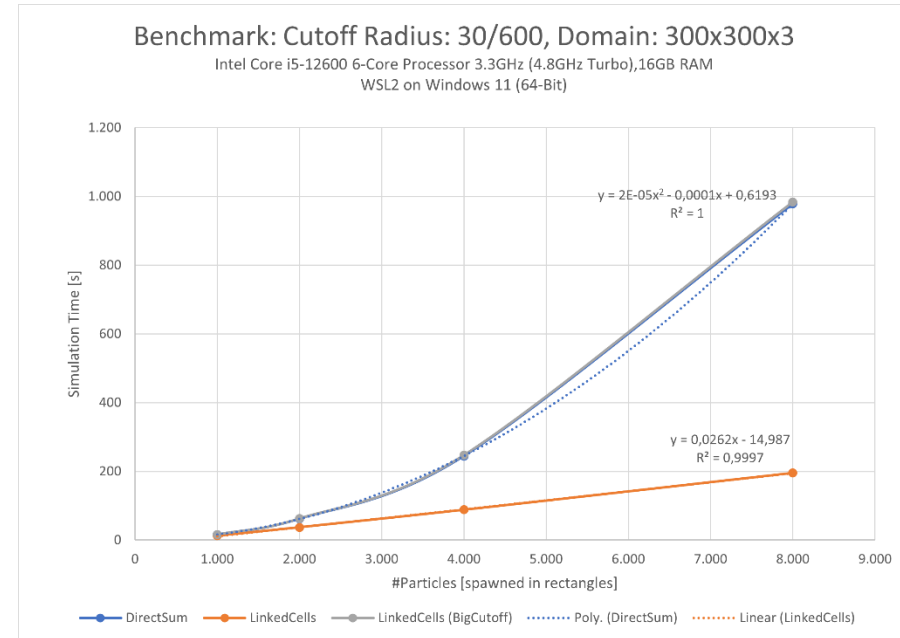


# Linked-Cells-Algorithm



# Linked-Cells-Algorithm

- **Performance:**
    - We tested on WSL and native Ubuntu
    - Direct sum container: Quadratic Growth
    - Linked Cells container: Linear Growth
- ⇒ Very good approximation

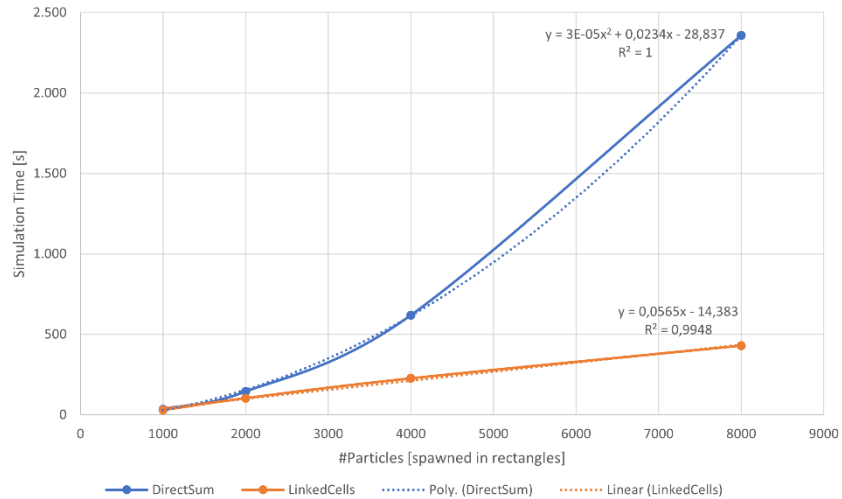




# Linked-Cells-Algorithm

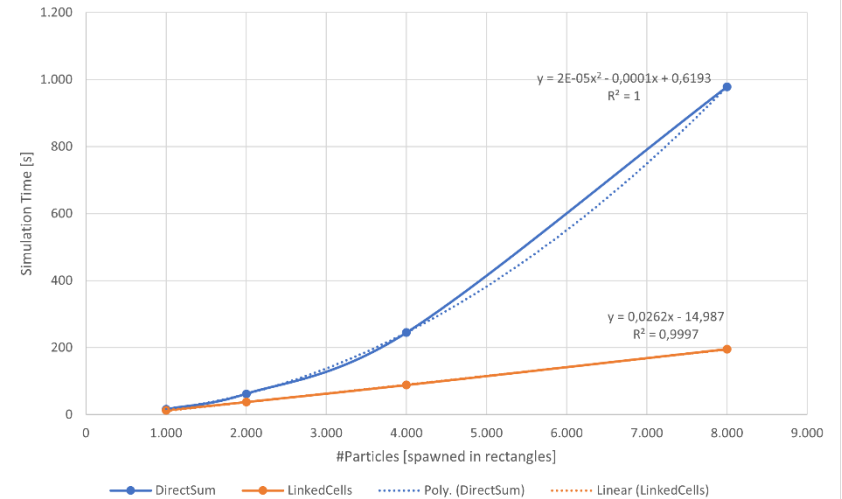
Benchmark: Cutoff Radius: 30, Domain: 300x300x3

AMD Ryzen 5 3600 6-Core Processor 3.59 GHz, 16GB RAM  
WSL2 on Windows 11 (64-Bit)



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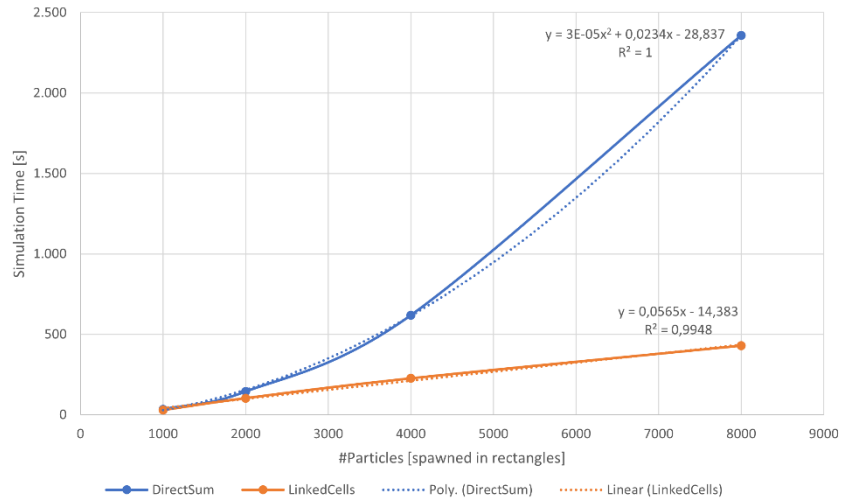
Intel Core i5-12600 6-Core Processor 3.3GHz (4.8GHz Turbo), 16GB RAM  
WSL2 on Windows 11 (64-Bit)



# Linked-Cells-Algorithm

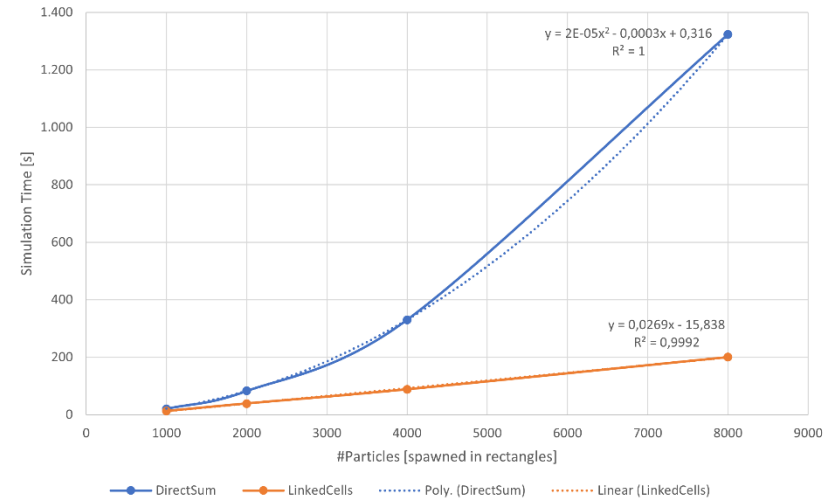
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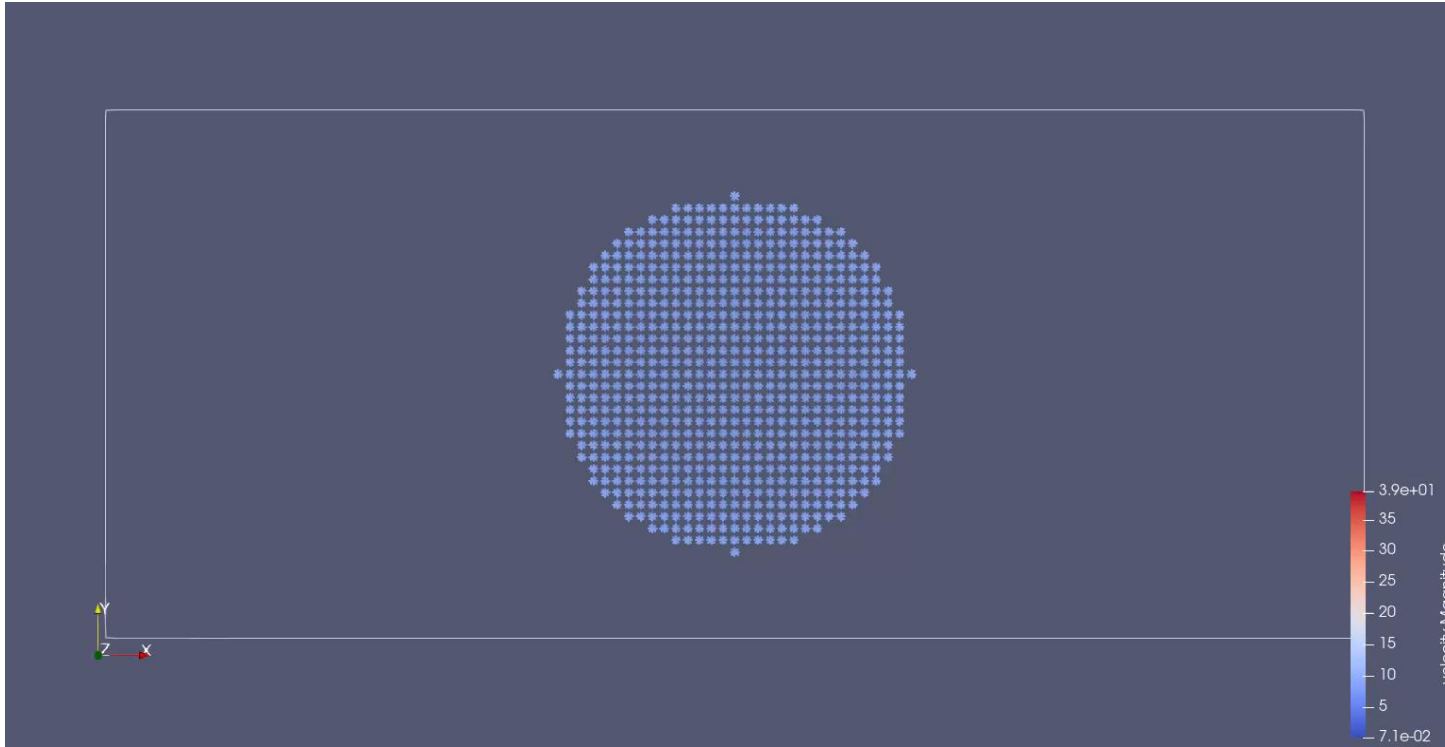


Benchmark: Cutoff Radius: 30, Domain: 300x300x3

Intel i5-10210U 4-Core Processor 1.6GHz (4.2GHz Turbo), 8GB RAM  
Ubuntu 22.04.3 LTS (64bit)



# Simulation of a falling drop - Wall

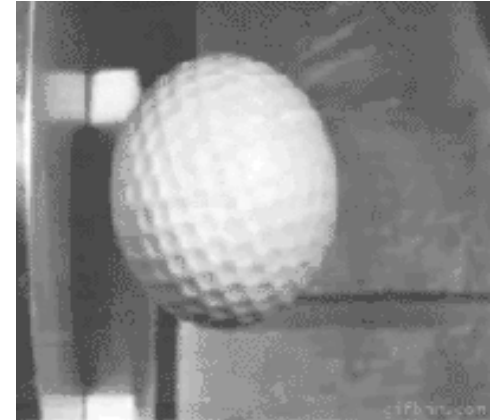


# Simulation of a falling drop - Wall

- **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 particles 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-Schnelladeanschluss-2016-2022-2018-2022-Wei%C3%9F/dp/B0BPJQYVQ3>

Golf ball collision: <https://gifer.com/en/gifs/collisions>

Our submission material hosted on Github Pages:

<https://manuellerchner.github.io/MolSim-WS23-24/submissions/>