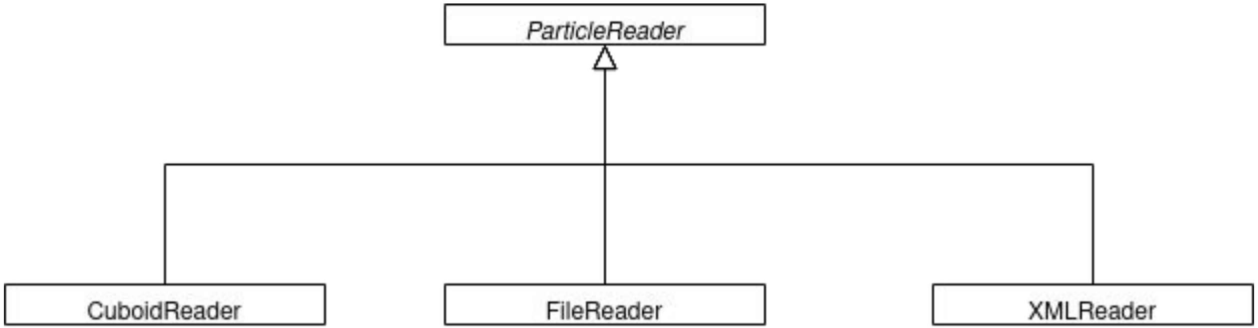
PSE Molekulardynamik

Team D - Sheet 3 : XML, Linked-cell algorithm and “falling drop - Wall”

Empowering Users: XML input

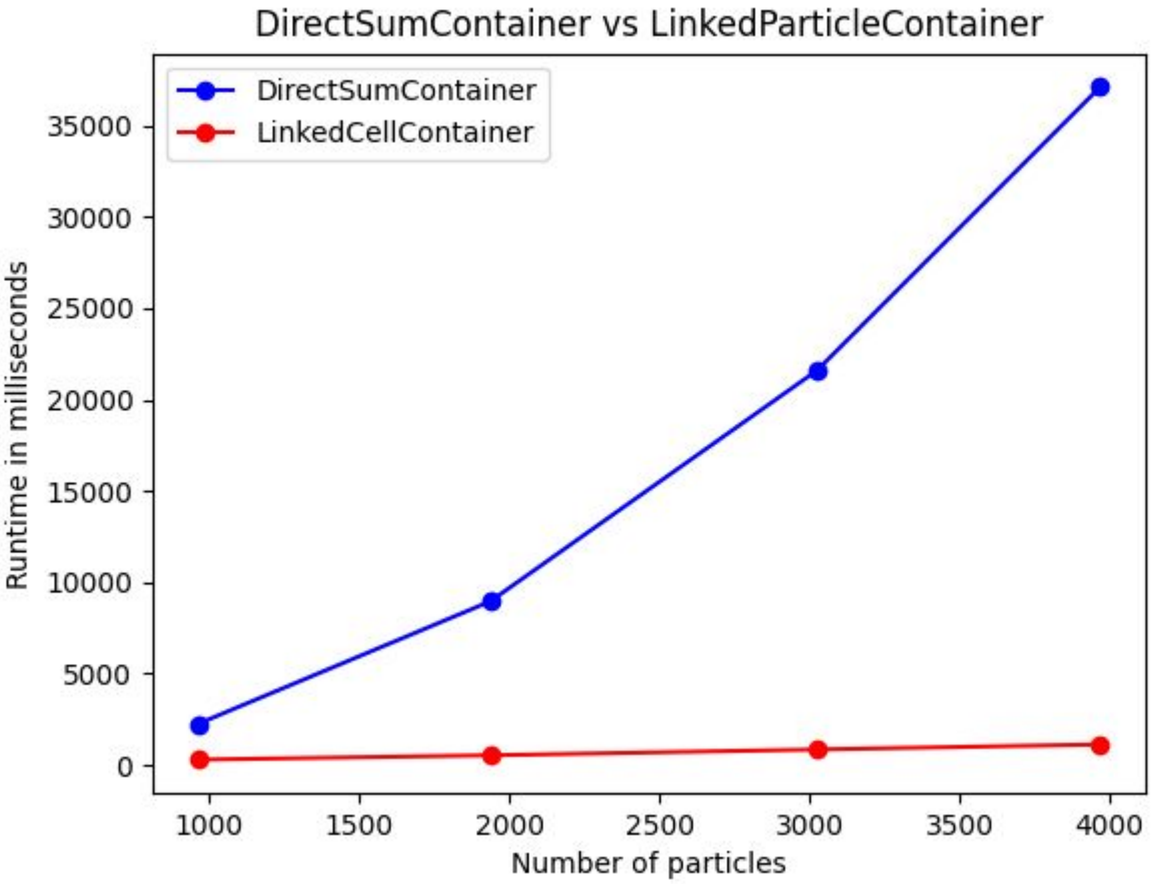
- Specification of input format through an xsd file
- more user friendliness for providing parameters and particles to the program



Implementing a new container

- We created a new ParticleContainer interface that summarizes our containers
- Type of container can be chosen at runtime
- We compared runtime of both containers as the number of particles increase:

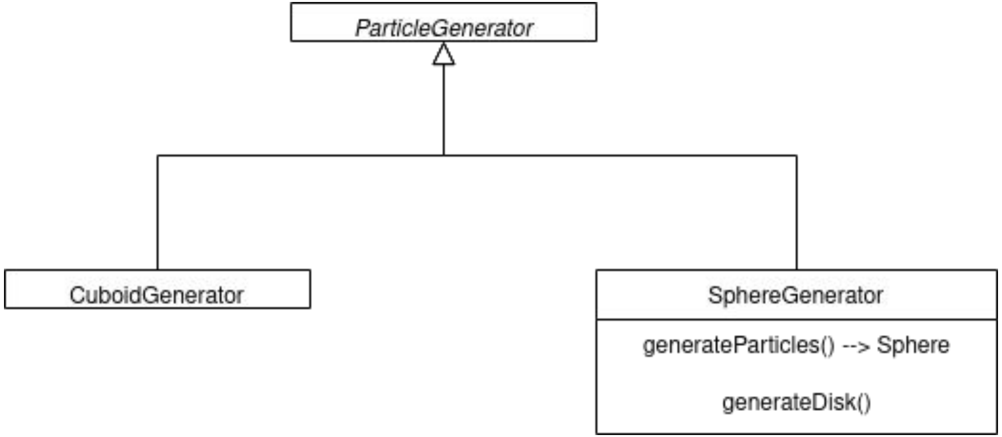
  see next slide


DirectSumContainer vs LinkedParticleContainer
DirectSumContainer
LinkedCellContainer
Runtime in milliseconds
0
5000
10000
15000
20000
25000
30000
35000
1000
1500
2000
2500
3000
3500
4000
Number of particles

Sphere Generation

- equation for a sphere and the calculation of distances to determine if a point lies within the sphere
- Equation of a Sphere with a center (a, b, c) and radius r is given by:

$$(x - a)^2 + (y - b)^2 + (z - c)^2$$



(healthy) Boundaries

Design idea

- Boundaries are a property of the linked cell algorithm
- But how and when boundaries are enforced depends on the simulation logic

As a consequence, a boundary class should implement the logic concerning boundary conditions, such as

- Which “walls” have which boundaries
- Dimensions and lower-left-corner

(healthy) Boundaries 2

Responsibilities of the simulation

- Go through each “wall” and apply expected boundary
- Maintain position consistency of particles inside simulation

→ Particles that go out of bounds should be deleted and ghost particles should not enter the simulation

Types of Boundary

1. Reflective - Force: The force of a ghost particle gets injected, but not particle gets added onto the simulation
2. Reflective - Particle: A particle gets effectively added onto the simulation and then discarded after the iteration
3. Outflow: Delete if outside

Boundaries: Considerations

Not a happy story…

- We couldn't really finish this part

But our expectations are that:

1. Reflective works best by using the ghost force
2. Outflow is more performant but may not be physically accurate

Particles Forming a Sphere