PSE Molecular Dynamics: Worksheet 3

Group C, 03.12.2024

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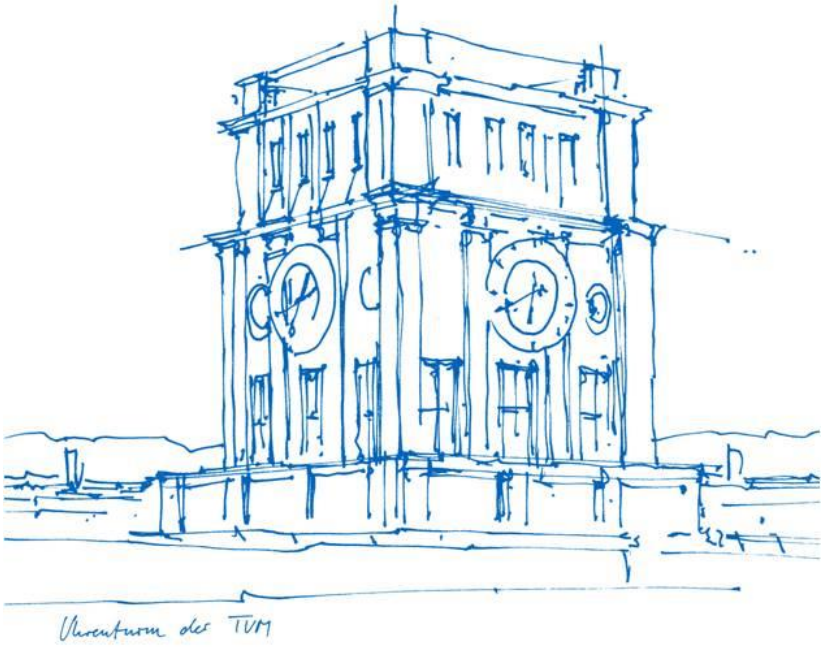


Now in glorious 4:3 Technicolor!

XML Input


```
<sim>
    <args>
        …
    </args>
    <type>lj</type>
    <totalParticles>486</totalParticles>
    <objects>
        …
    </objects>
</sim>
```

XML Input

```
<sim>
    <args>
        …
    </args>
    <type>lj</type>
    <totalParticles>486</totalParticles>
    <objects>
        …
    </objects>
</sim>
```

Optional arguments passed in here…

XML Input

```
<sim>
    <args>
        …
    </args>
    <type>lj</type>
    <totalParticles>486</totalParticles>
    <objects>
        …
    </objects>
</sim>
```

Specify simulation type…

XML Input

```
<sim>
    <args>
        …
    </args>
    <type>lj</type>
    <totalParticles>486</totalParticles>
    <objects>
        …
    </objects>
</sim>
```

XML Input

```
<sim>
    <args>
        …
    </args>
    <type>lj</type>
    <totalParticles>486</totalParticles>
    <objects>
        …
    </objects>
</sim>
```

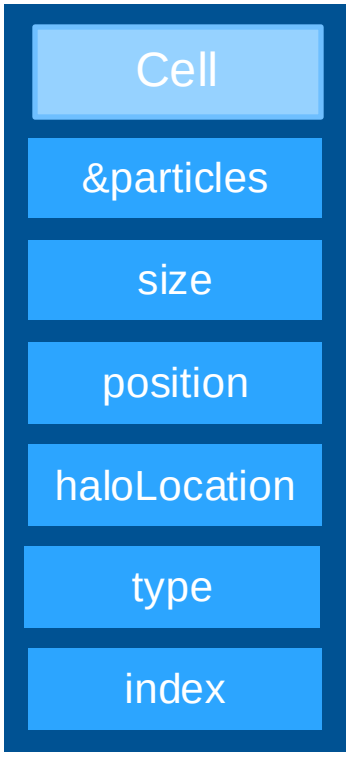
Linked Cells Algorithm

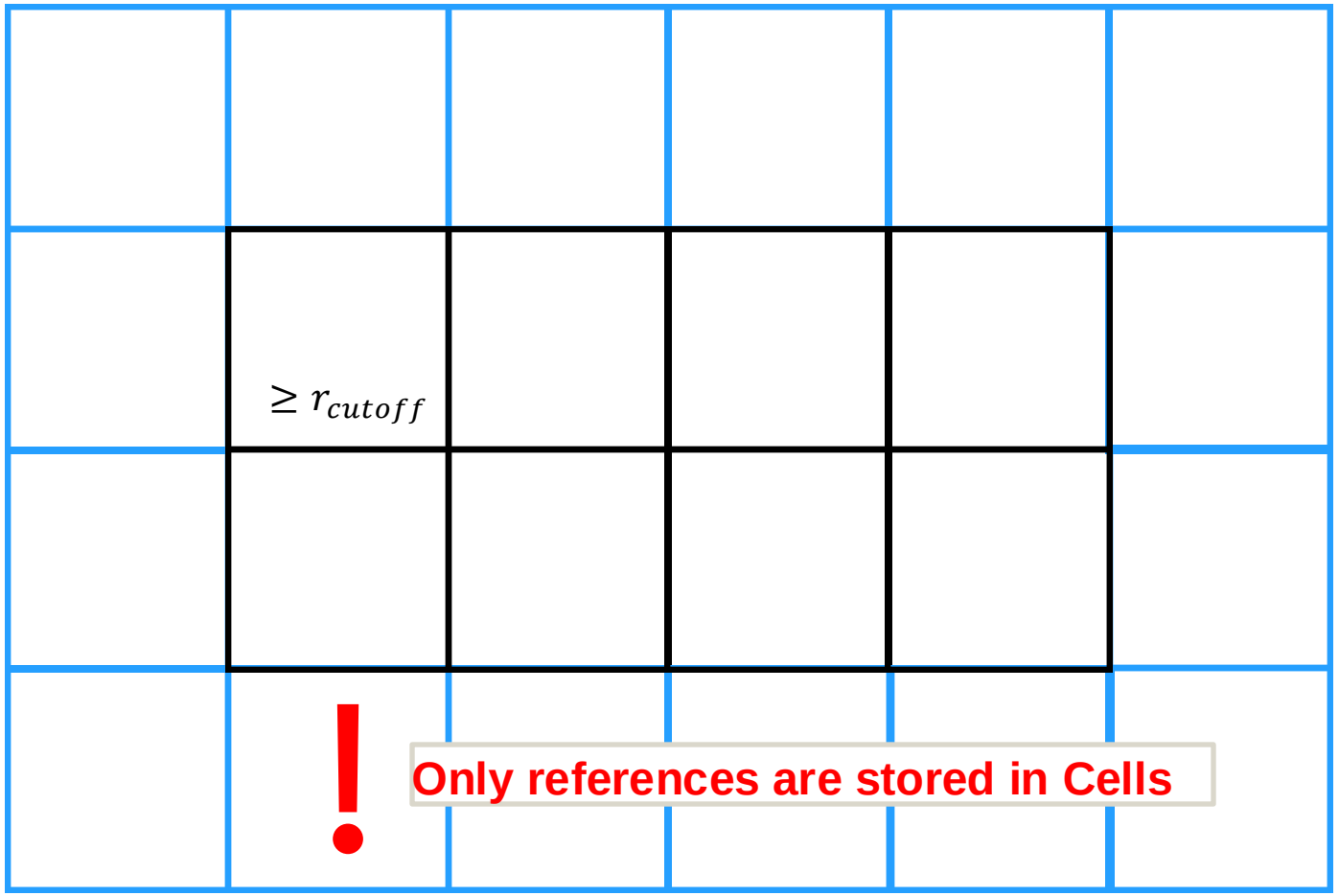
Split the domain into equally sized cells

Halo Cells

Border Cells

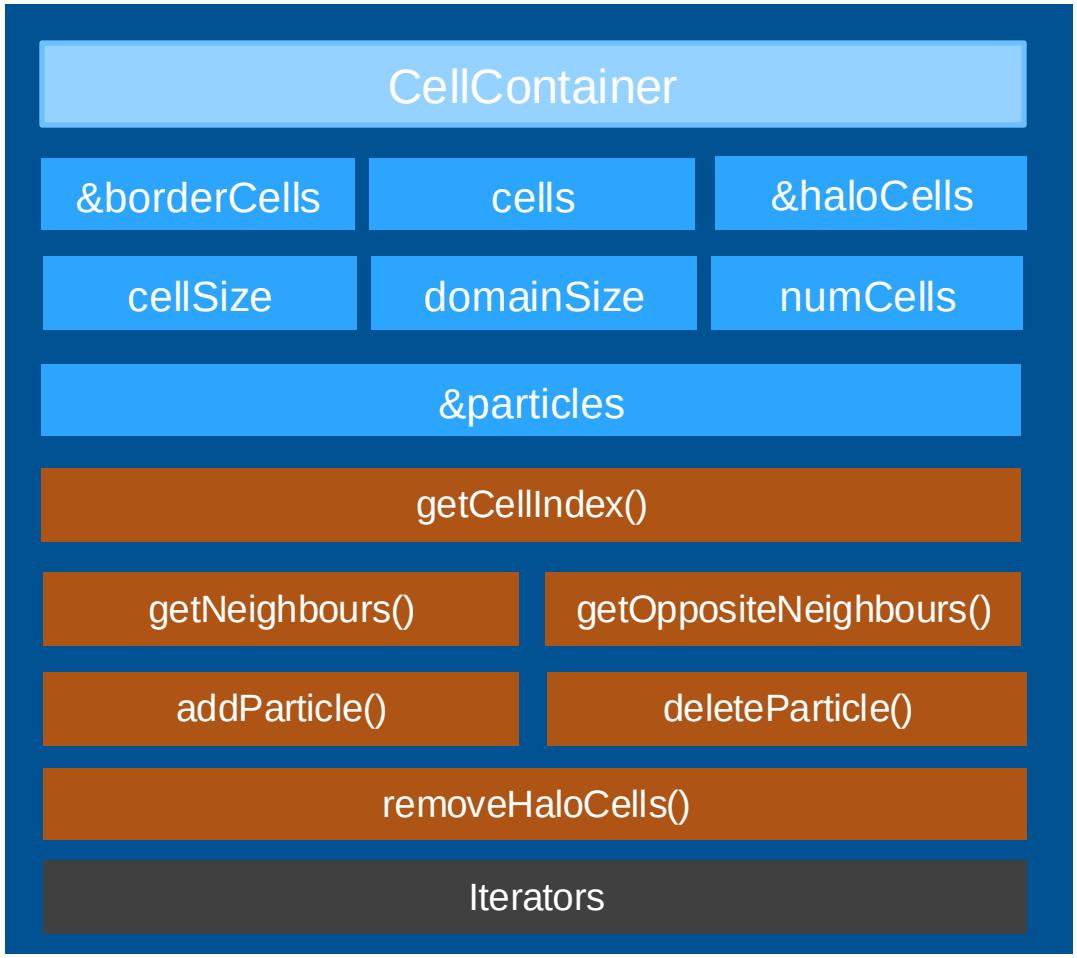
Inner Cells





CellContainer

Manager Class for Cells



Initialization

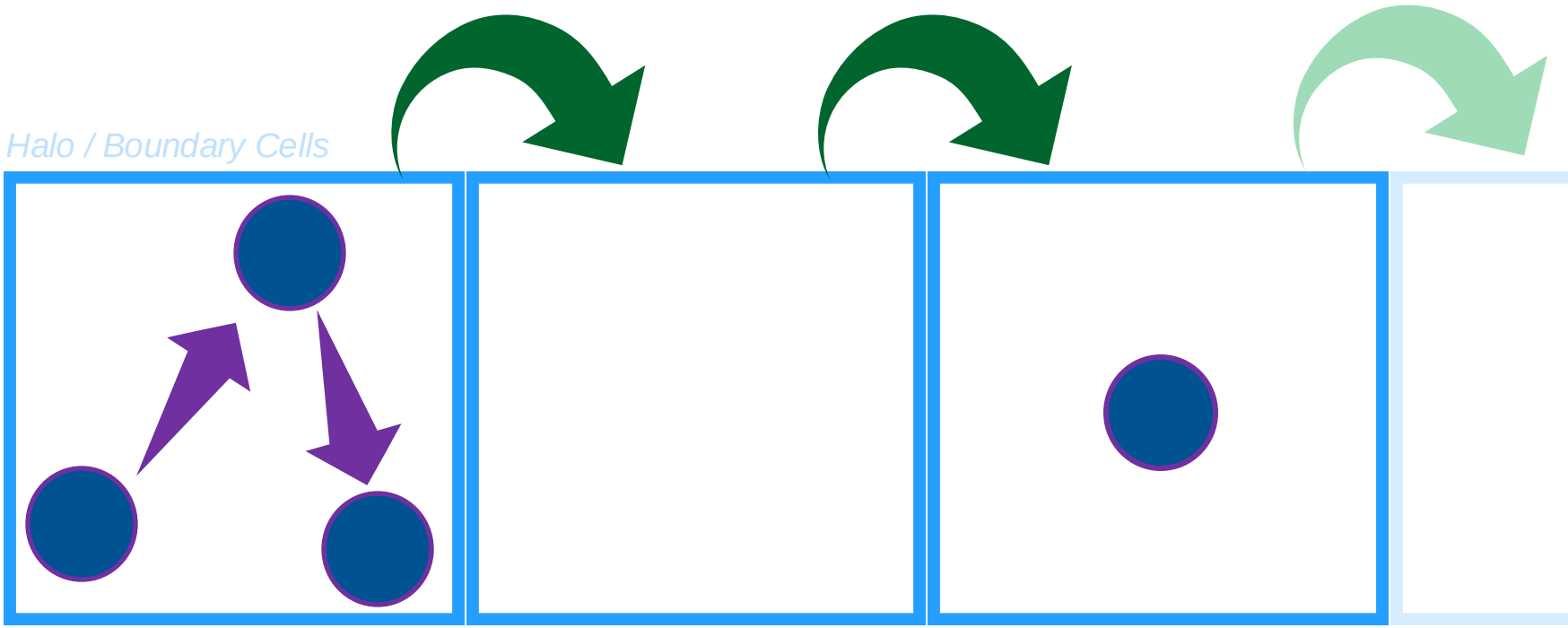
create Cells
determine their attributes
add the particles

Basic Functionality

finding neighboring cells
moving particles between cells
removing particles in Halo
iterators

+ minor functions and QOL additions

Iterators



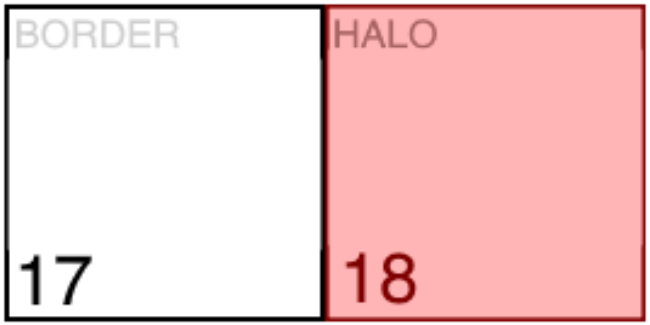
Inner: Iterates over the particles in a cell.

Outer: Iterates over the cells; *skips empty cells*.

Collision of Two Bodies (Outflow) (Video)

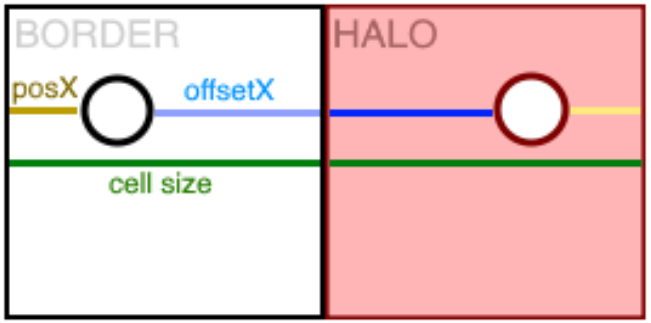
Collision of Two Bodies (Reflective) (Video)

Boundary Conditions (Reflective)



Component 1

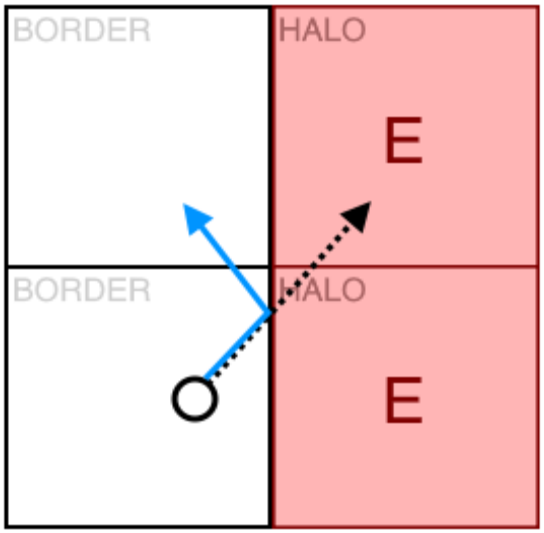
Finding the opposite neighbor of a cell

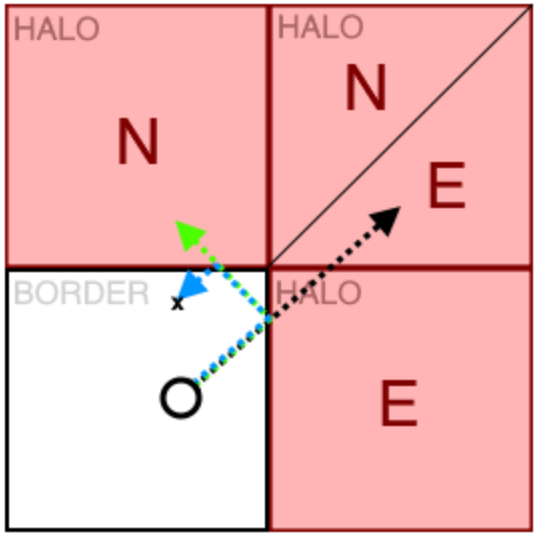


Component 2

Mirroring the particle position

Boundary Conditions (Reflective)

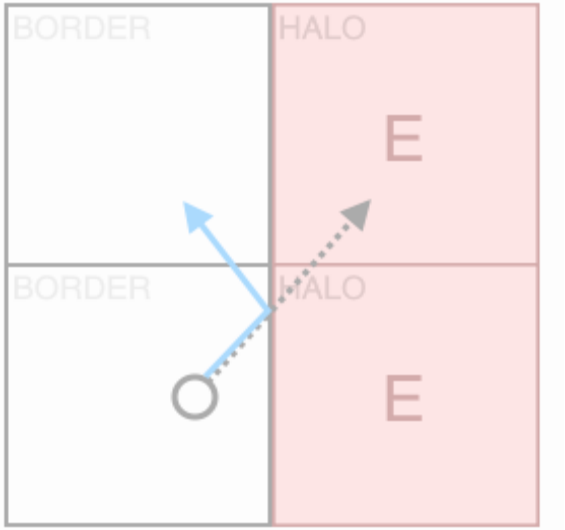


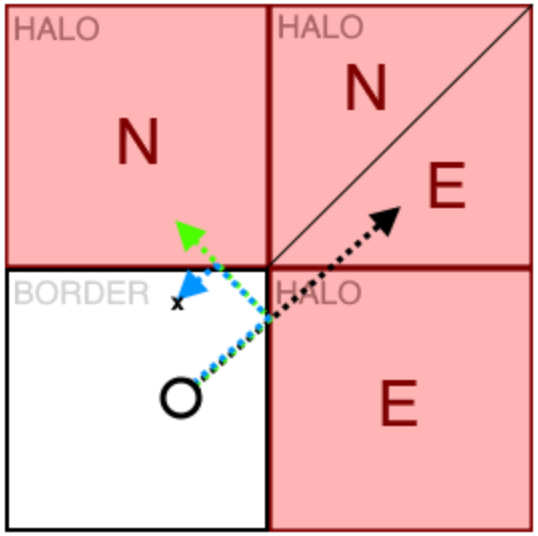


When a particle enters a reflective halo cell:

1. Find the opposing cell.
2. Mirror the particle position.

Boundary Conditions (Reflective)

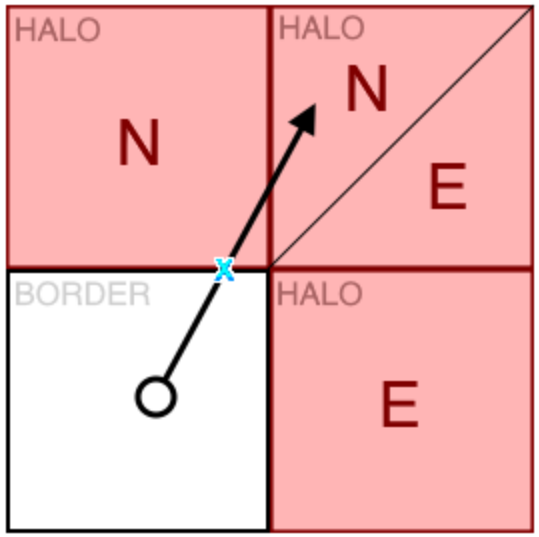


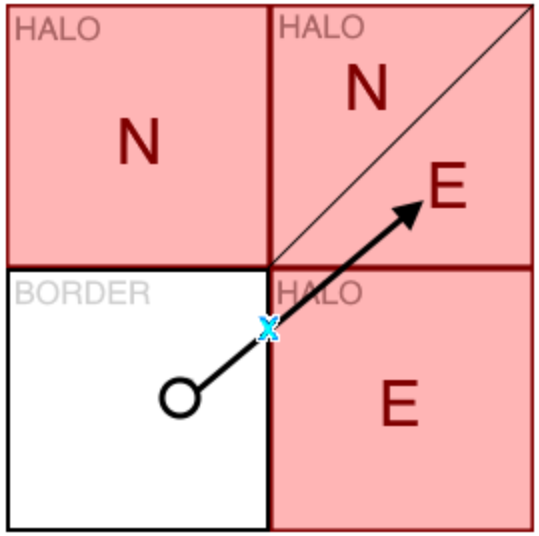


How do we know which boundary condition to apply for **corner halo cells?**

E outflow, **N** reflective, which to choose?

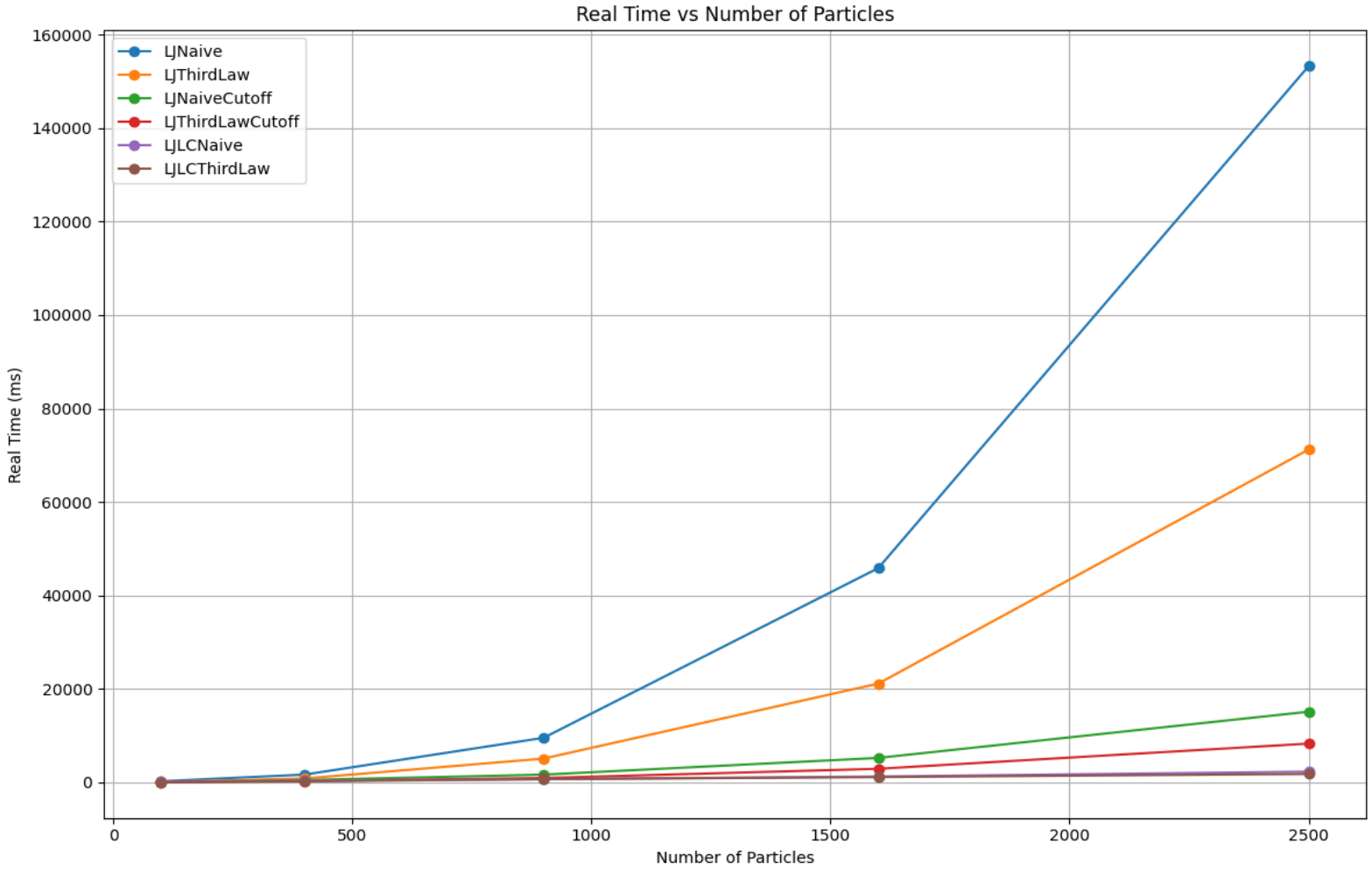
Boundary Conditions (Reflective)



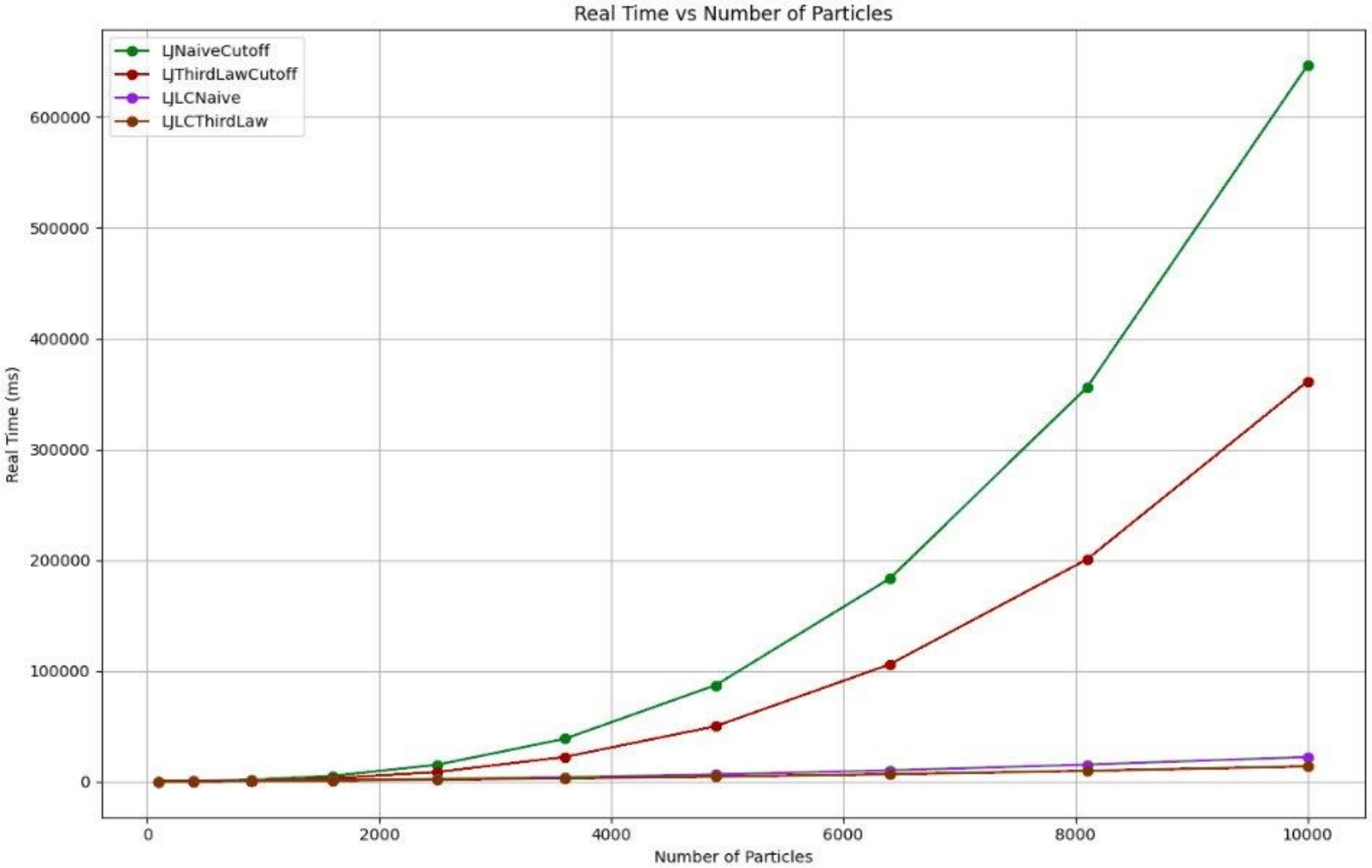


Divide the corner cell in **two**,
then check if the particle is **above or below** the line

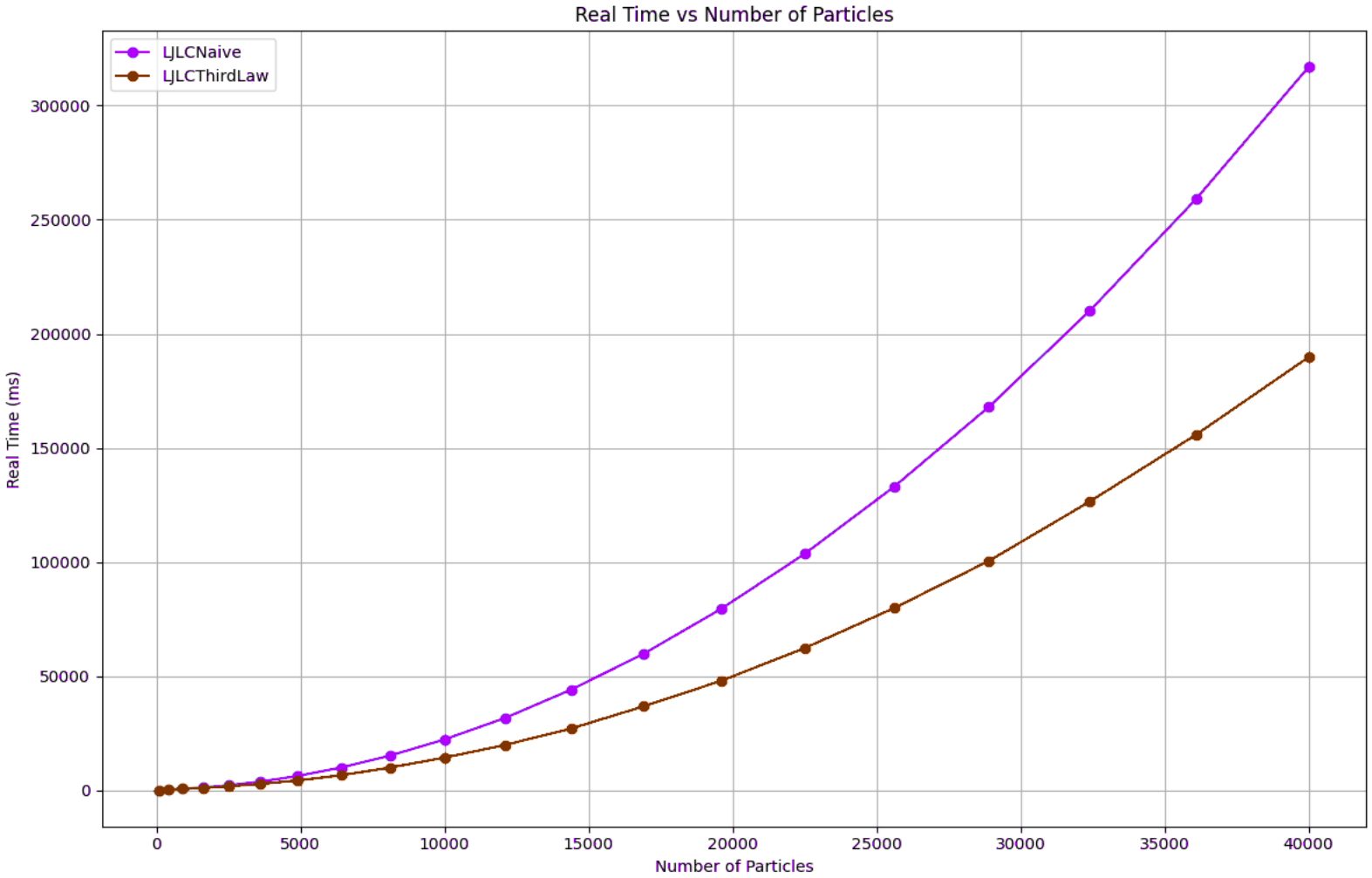
Benchmarking (All Implementations)



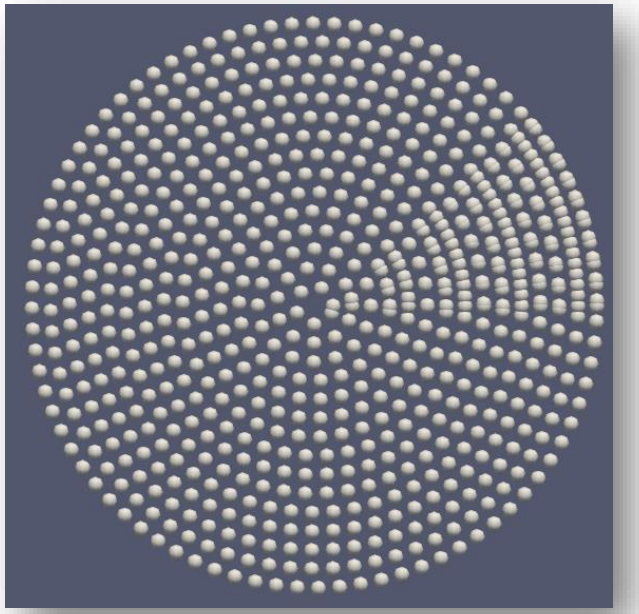
Benchmarking (Cutoff Implementations)



Benchmarking (Linked Cells)



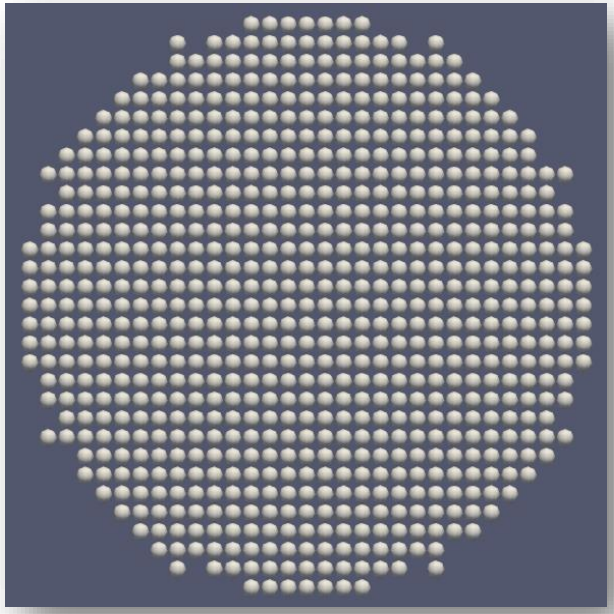
2D Spheres



Approach 1

Concentric Circles

overlap, not a grid

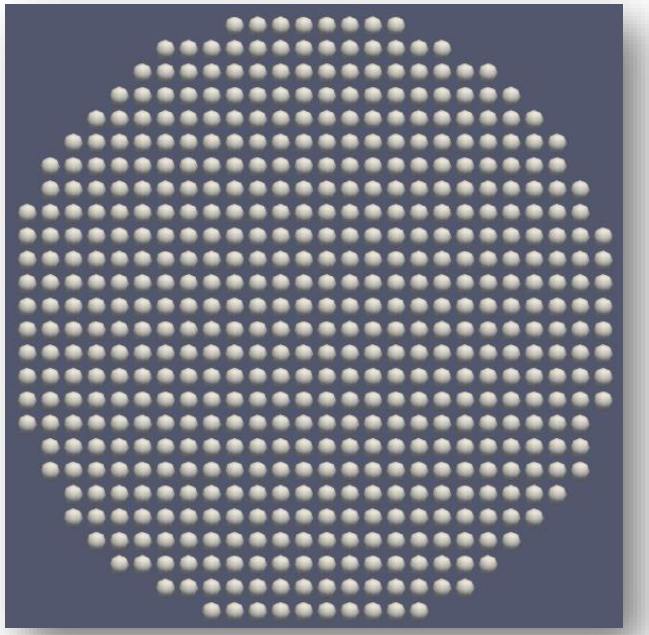


Approach 2

Midpoint Circle Algorithm

messy borders, buggy

2D Spheres



Approach 3

Simple Iterative Algorithm

Falling Drop Simulation (Video)