PSE Molecular Dynamics: Worksheet 4

Group C, 20.12.2024

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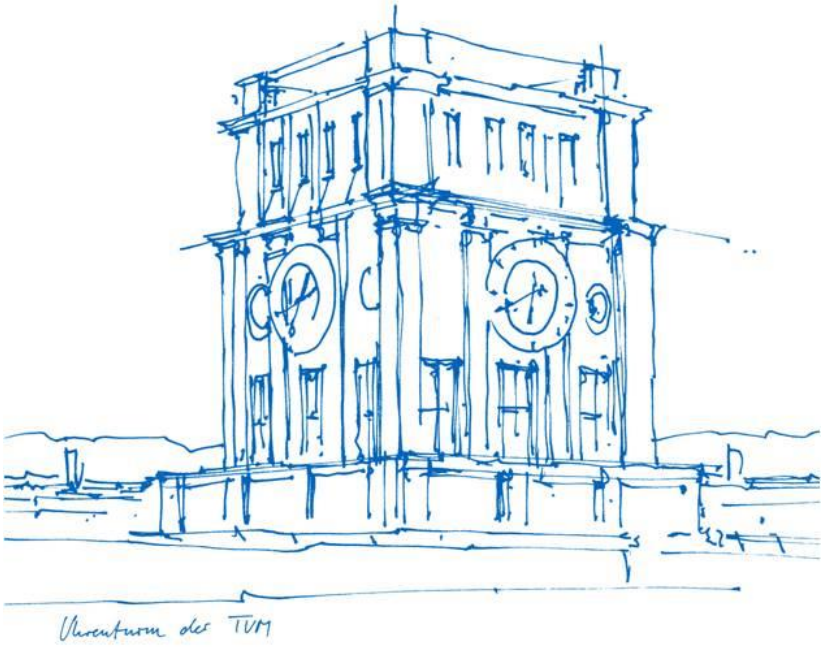
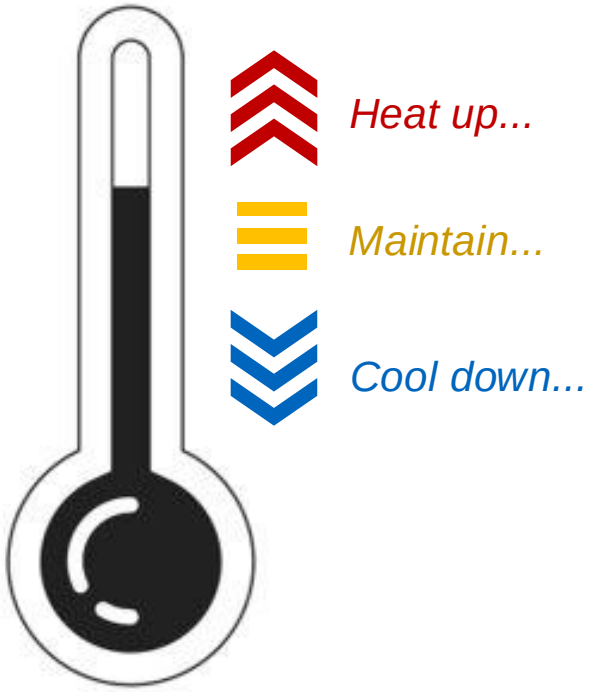


Thermostat



- Calculate **kinetic energy**
- Derive **current temperature** from kinetic energy
- Calculate **scaling factor** to be applied on particle velocities

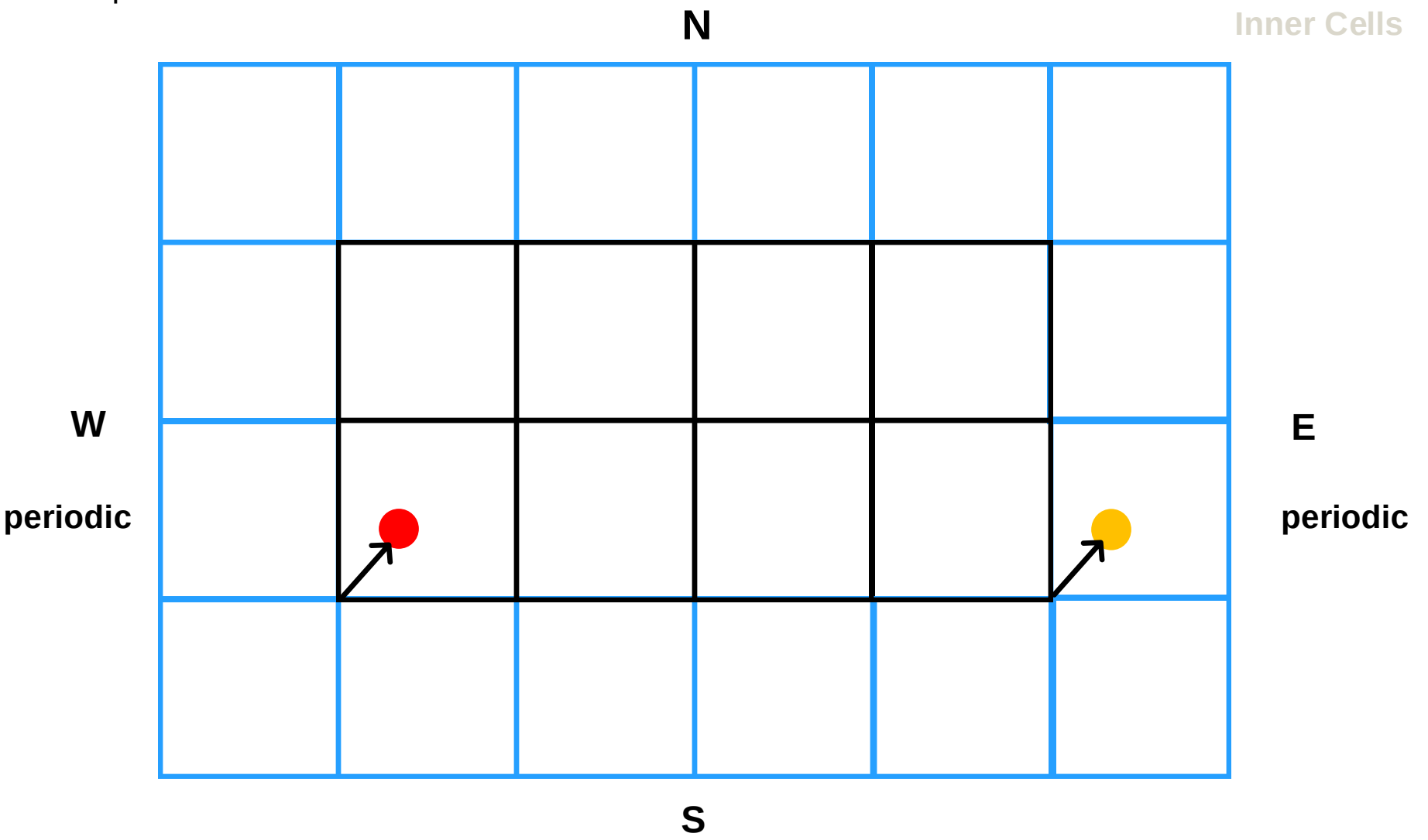
Periodic Boundaries - Movement

Move particles in Halo based on cardinal direction

Halo Cells

Border Cells

Inner Cells



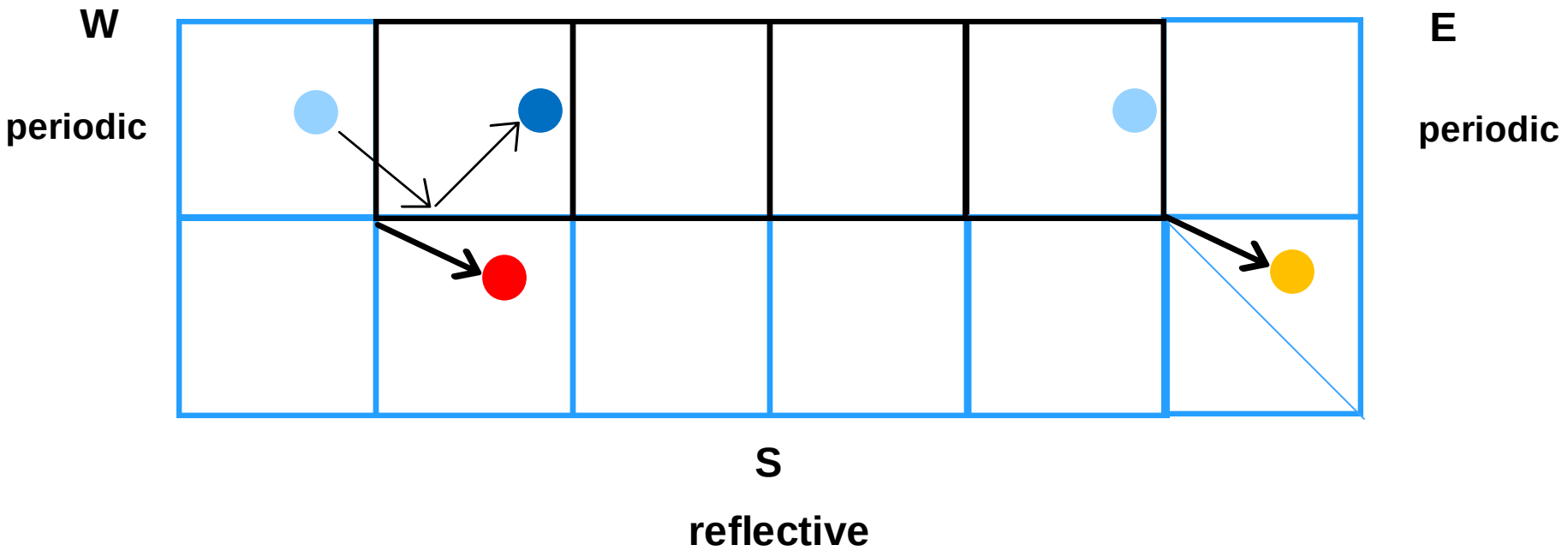
Periodic Boundaries - Movement

Special Corner Case

Halo Cells

Border Cells

Inner Cells



1. Apply periodic condition
2. Apply reflective condition

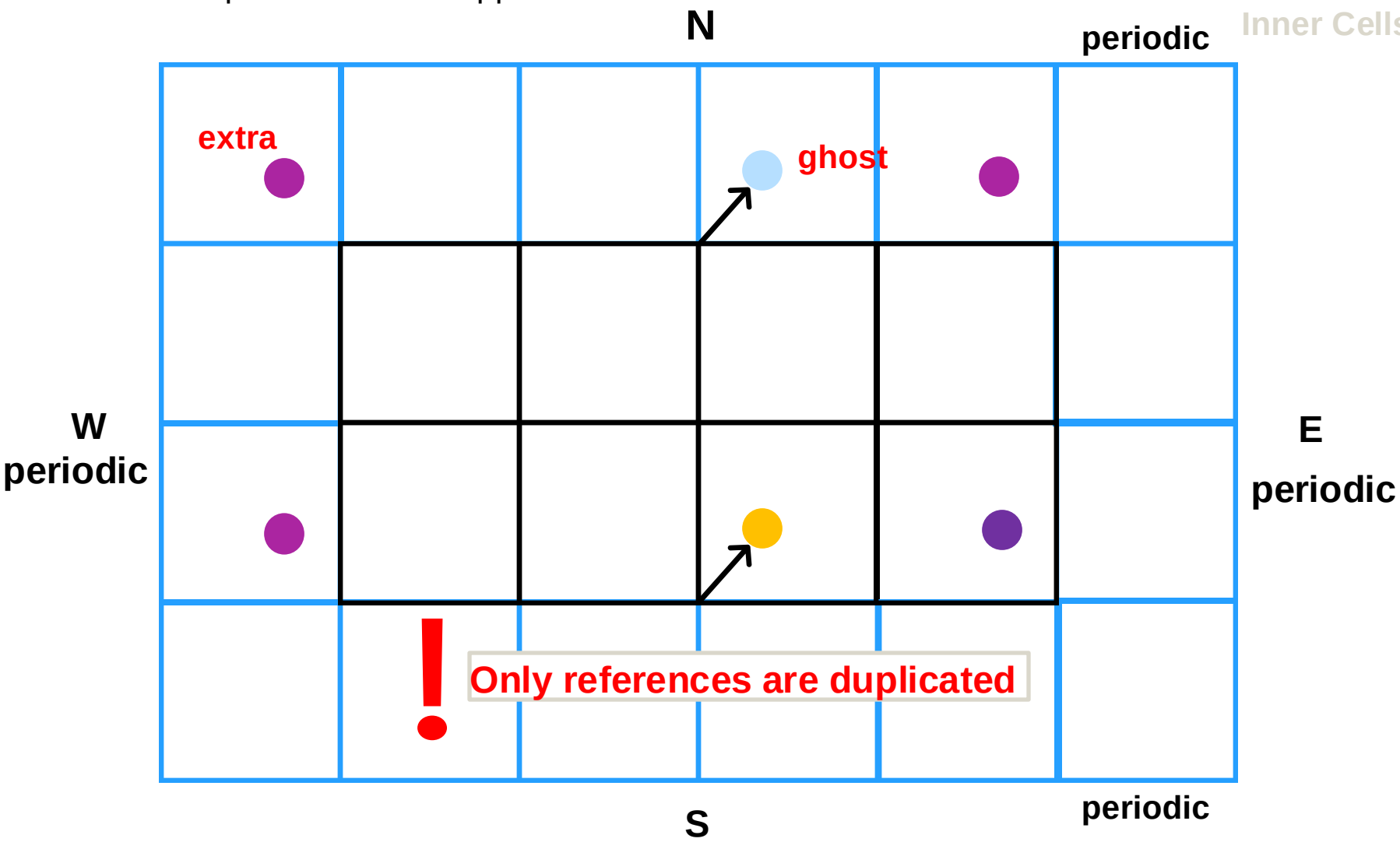
Periodic Boundaries – Ghosts

Mirror border particles on the opposite side of the domain

Halo Cells

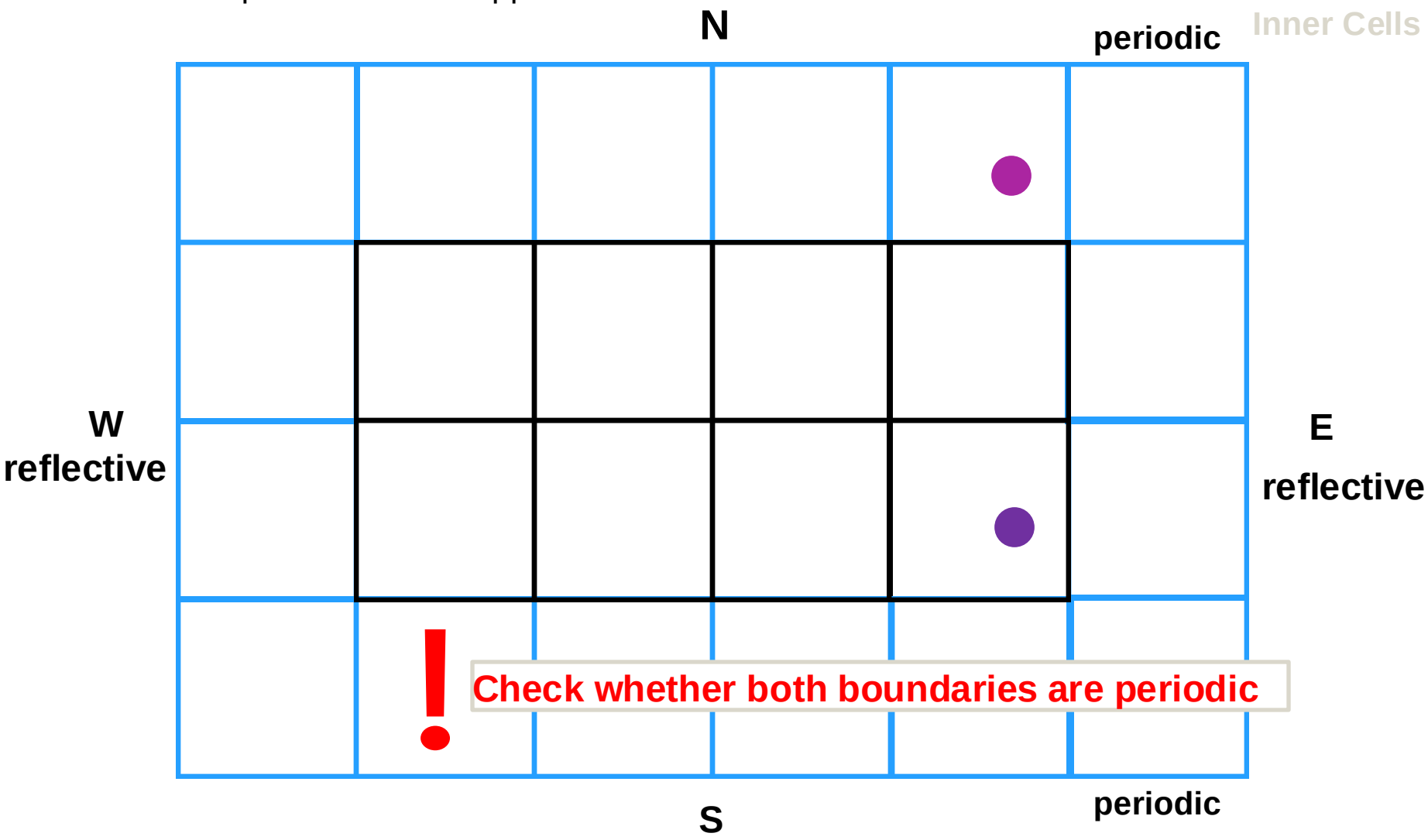
Border Cells

Inner Cells



Periodic Boundaries – Ghosts

Mirror border particles on the opposite side of the domain



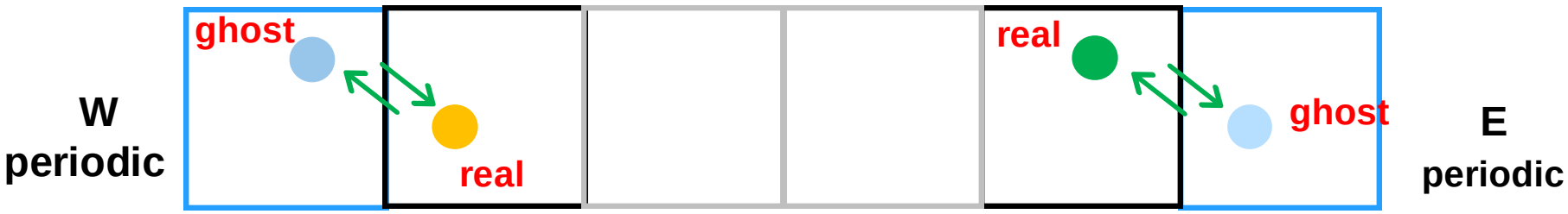
Periodic Boundaries – Ghosts

Use the ghost to calculate forces

Halo Cells

Border Cells

Inner Cells



Since all border particles are mirrored, we use normal third-law

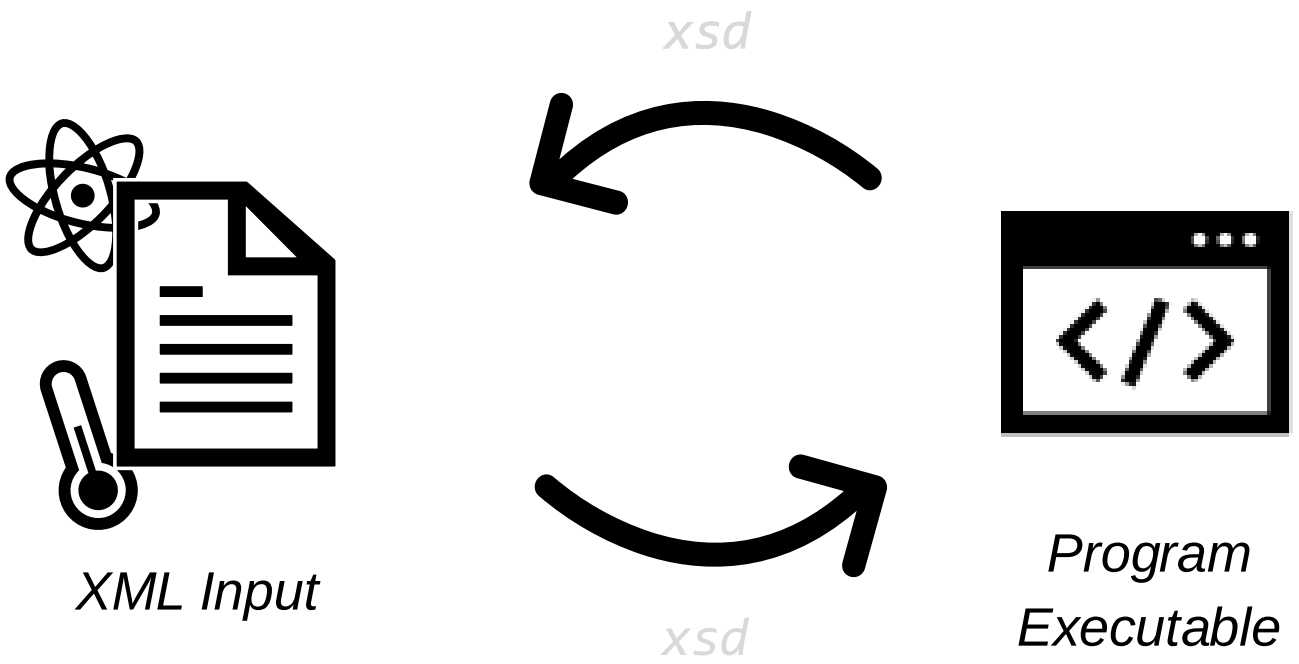
Skip over halo cells, otherwise forces are falsely multiplied!

S

Rayleigh-Taylor (Large) (Video)

(We also implemented gravitational forces)

Checkpointing



Falling Drop (Video)

Benchmarking

RELEASE build, -O3, I/O turned off.

Iterations	Runtime	MUPS
20000	397.9s (6.6min)	502675.5
50000	1008.6s (16.8min)	495768.7
100000	**2156.9s (35.9min)**	**463631.4**

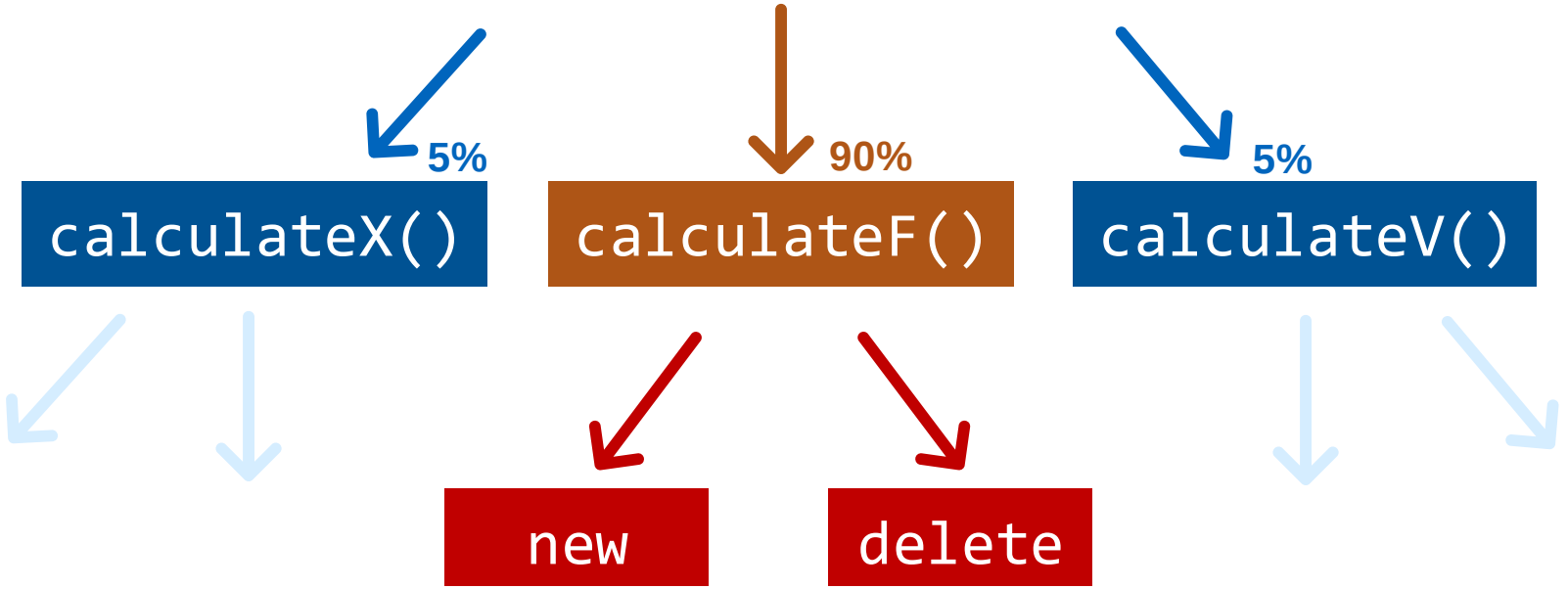
Runtimes on CoolMUC-4 for different iteration counts.

Compiled using G++ 7.5.0.

Compiler	Runtime	MUPS
`g++ 13.2`	899.1s (14.9min)	556131.4
`clang++ 16.0.2`	879.3s (14.6min)	568622.2
`icpx 2023.2.1`	**723.6s (12.1min)**	**691001.4**

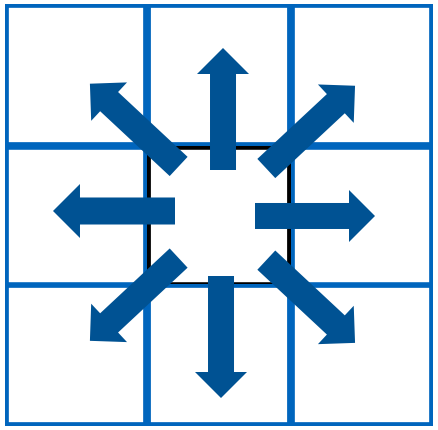
Runtimes on CoolMUC-4 for different compilers.

Profiling (gprof, callgrind)



As expected, force calculation takes up the most runtime...
...but there's also some unexpected heap allocations.

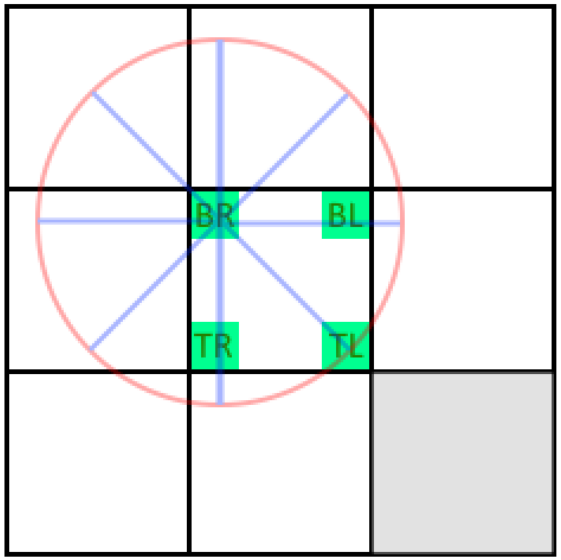
Optimizations (Successes)



Precomputing
Cell Neighbors
-1.5s

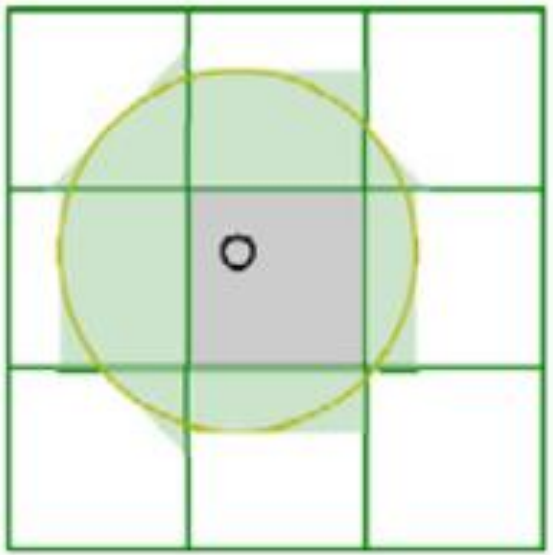
Removing
Inactive Particles
-1.3s

Optimizations (Failures)



Skipping Corner Neighbors

Too much overhead...



Gonnet's Algorithm

Out of time...