MolSim WS 23/24

Sheet 5

Membranes, Parallelization, Contest No.2,

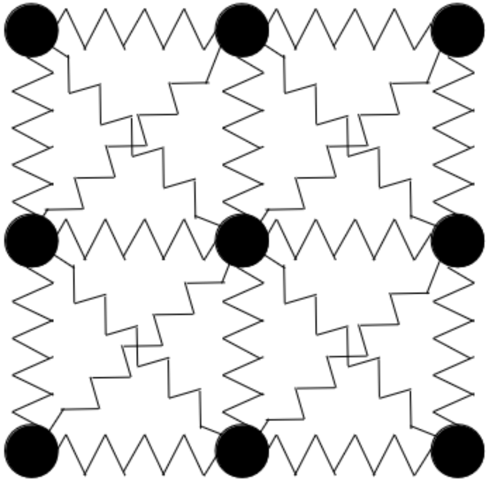
Nano-scale flow and Crystallization of Argon

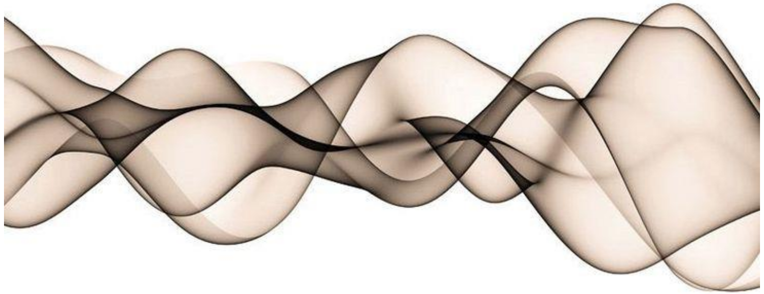
Group C [Manuel, Tobias, Daniel]

02.02.2024

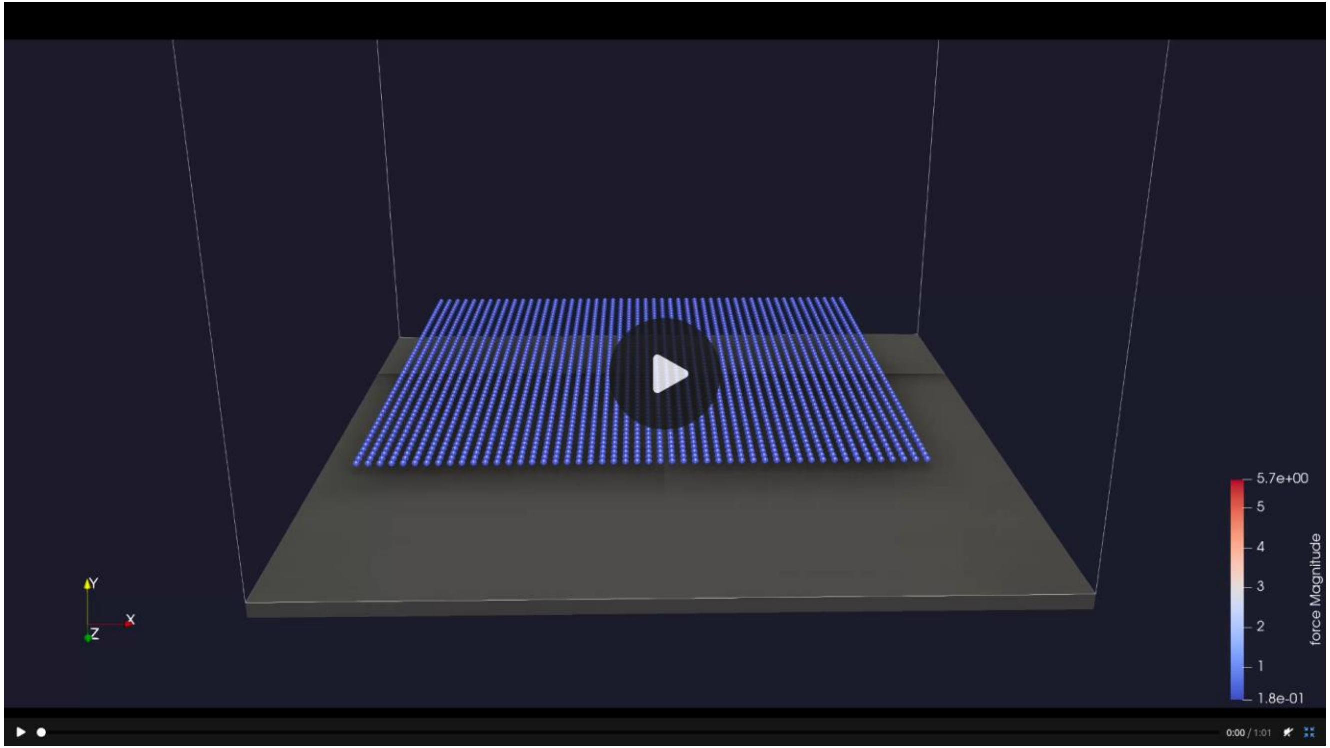
Simulation of a membrane

- **Harmonic Force**
  - ⇒ save neighbors for each particle
  - ⇒ save spring constant k
- **The temporary force**
  - ⇒ acts on selected set of particles
  - ⇒ acts for a specified amount of time
- **No Outflow boundaries**

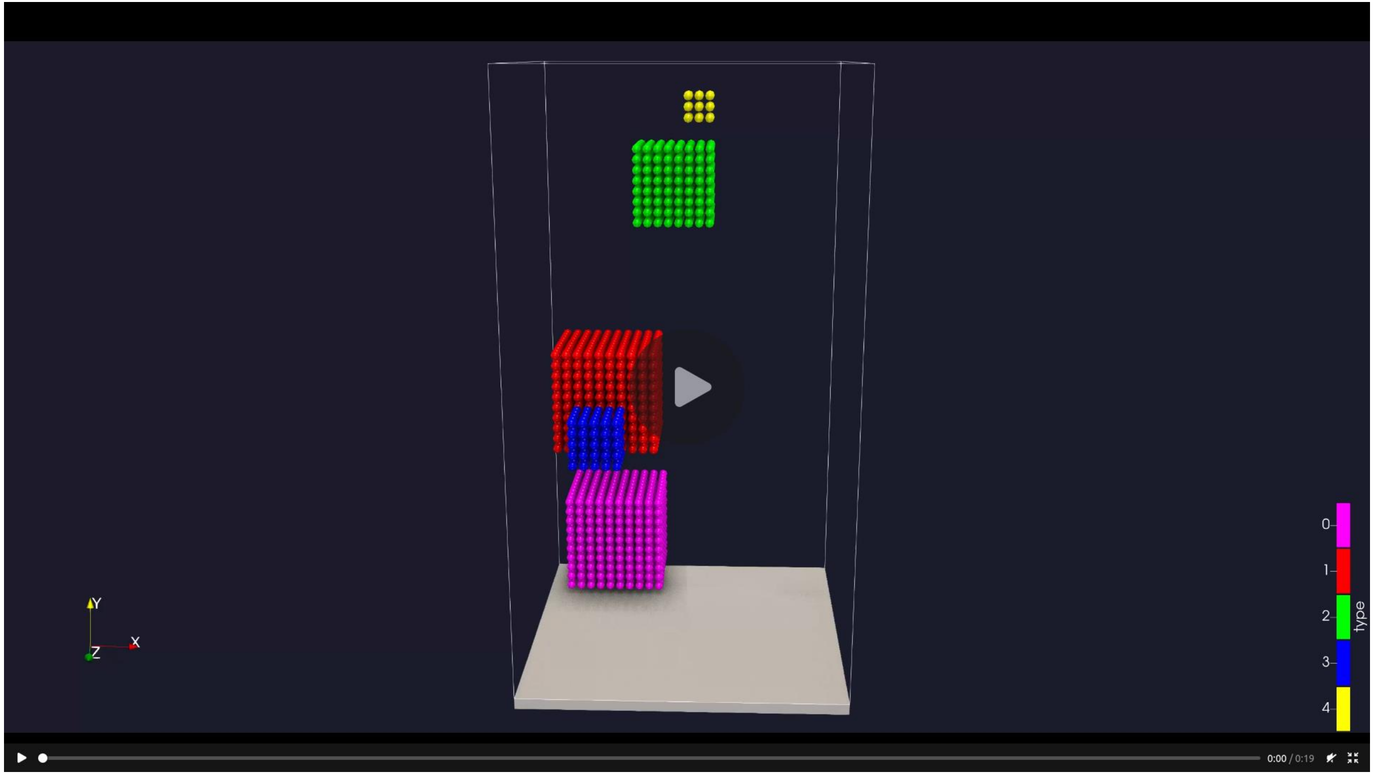




Simulation of a membrane



Simulation of a membrane



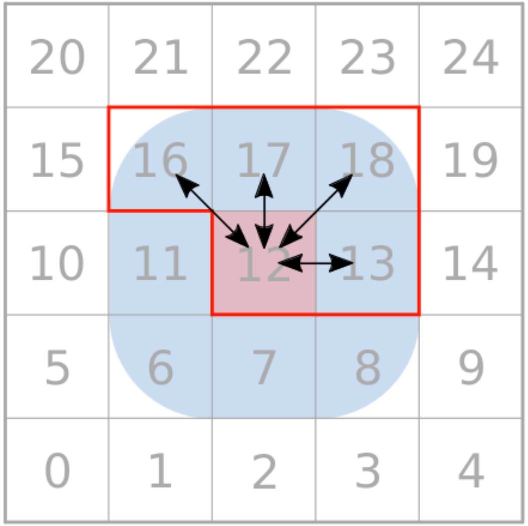
Parallelization

Domain Partitioning

- **Domain partitioning:**
  - Parallelization works on a linearized queue of list of Cells

    ⇒ this queue differentiates the 2 methods
  - All members of 1 list can be worked on in parallel without race conditions

    ⇒ deterministic result

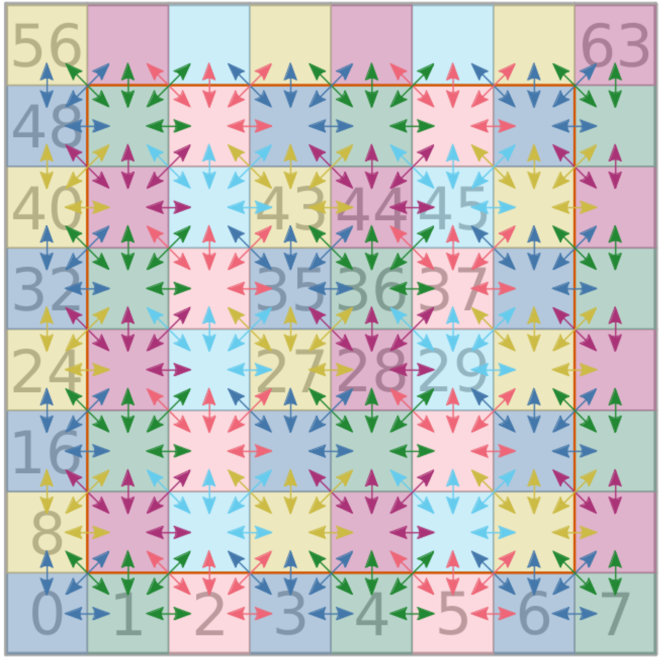


(b) c18 base step

Parallelization

Domain Partitioning

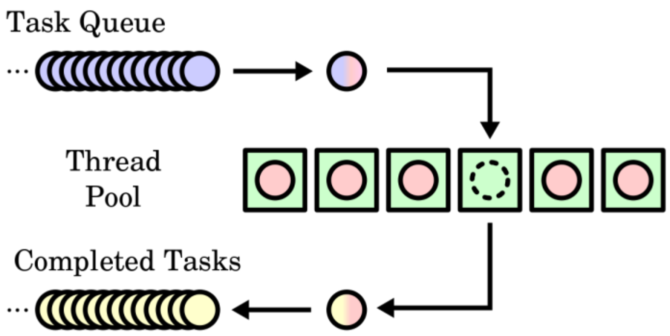
- **Domain partitioning:**
  - Parallelization works on a linearized queue of list of Cells
    ⇒ this queue differentiates the 2 methods
  - All members of 1 list can be worked on in parallel without race conditions
    ⇒ deterministic result
    ⇒ faster than second method



Parallelization

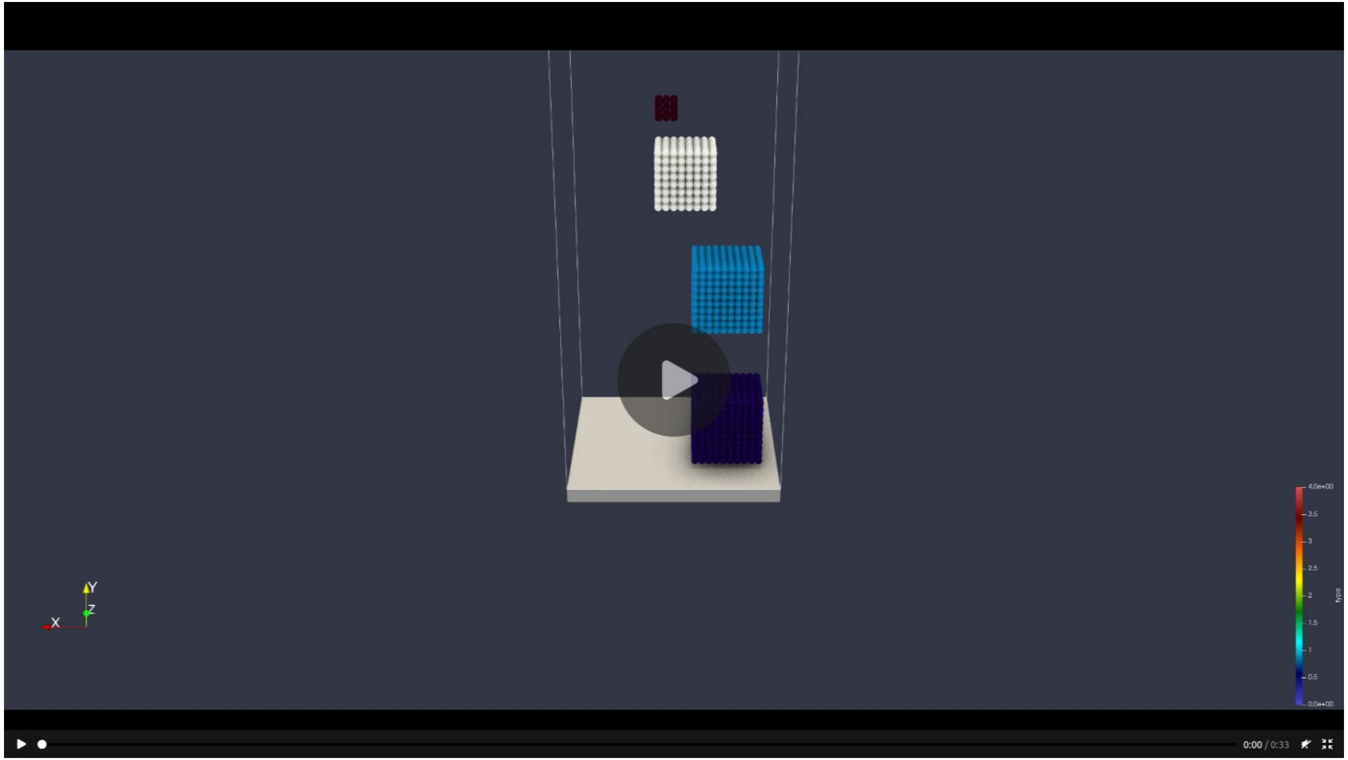
Particle Locking

- **Particle Locking:**
  - Mutexes on the level of particles
  - The list of cells in our queue is sorted randomly
  - ⇒ very little idle time in big examples because of randomization
  - ⇒ not deterministic
  - ⇒ order of calculation matters a lot in chaotic systems

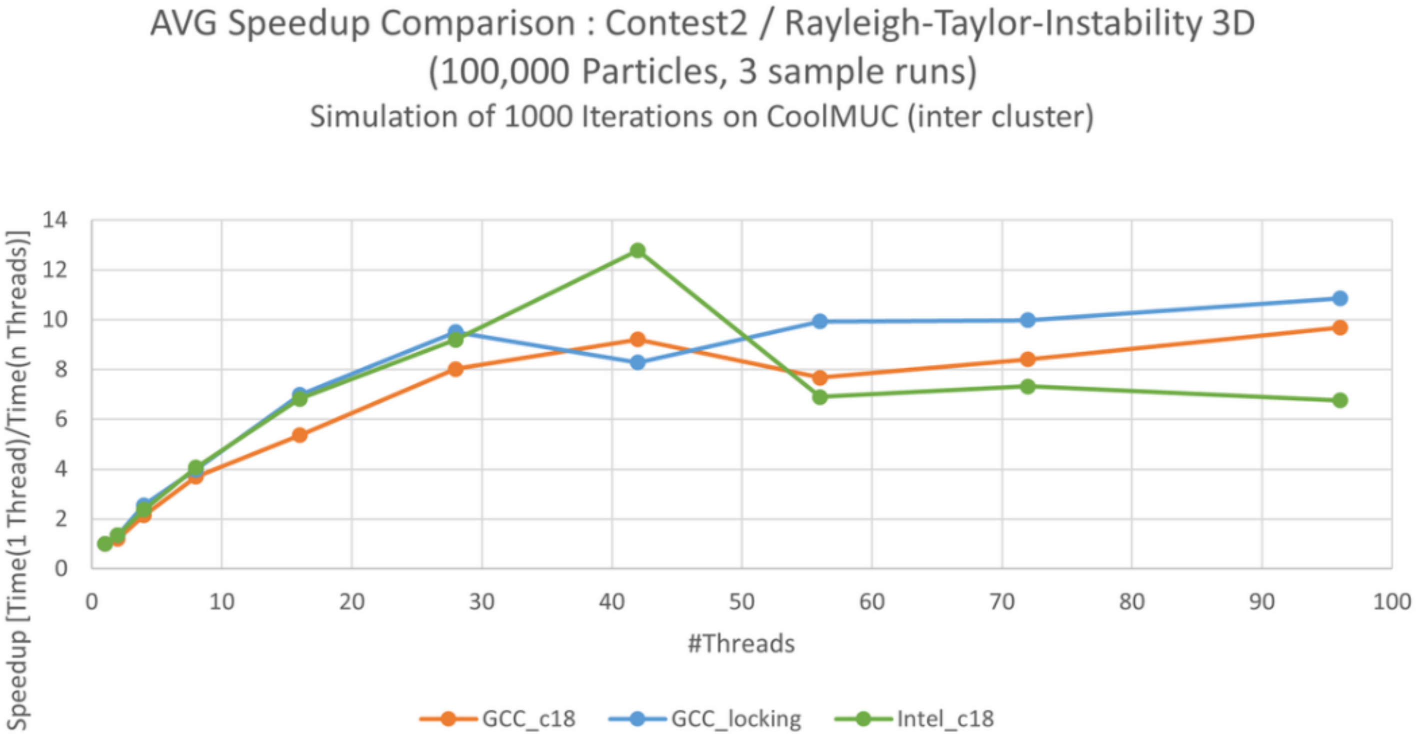


Parallelization

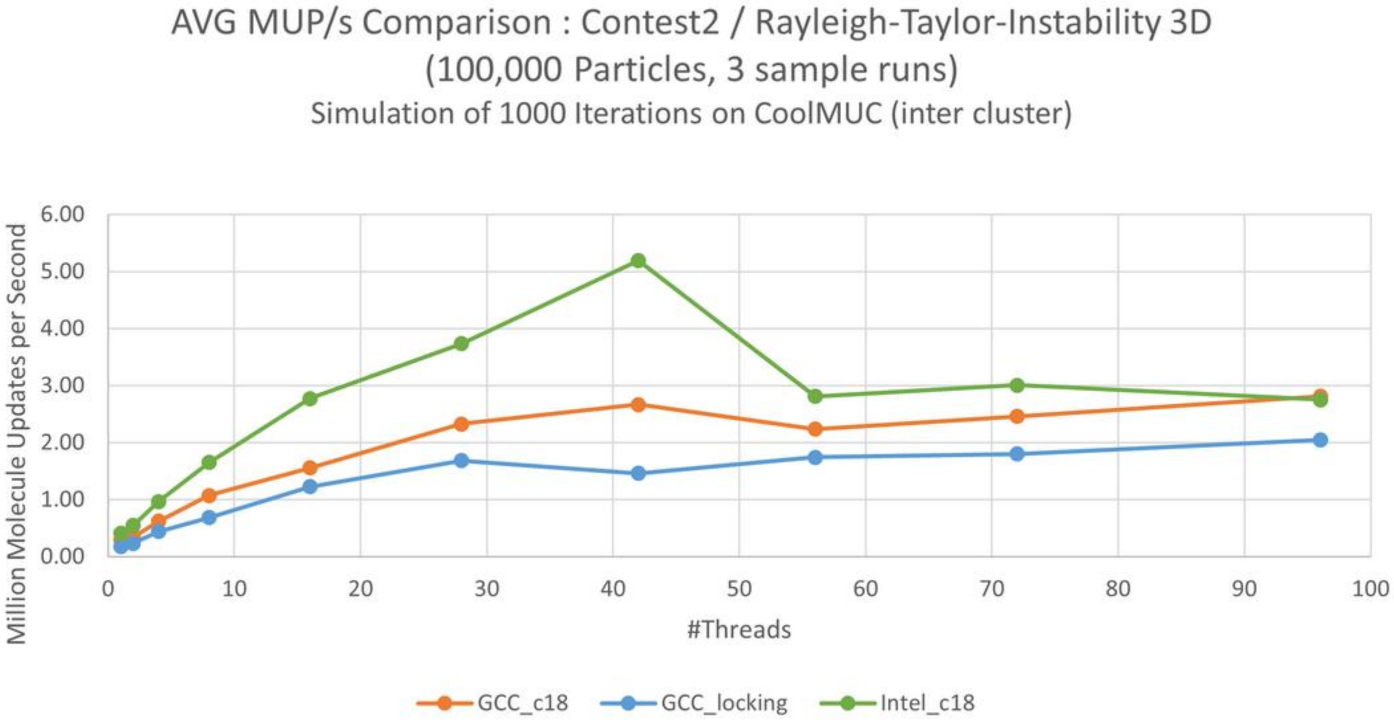
Particle Locking



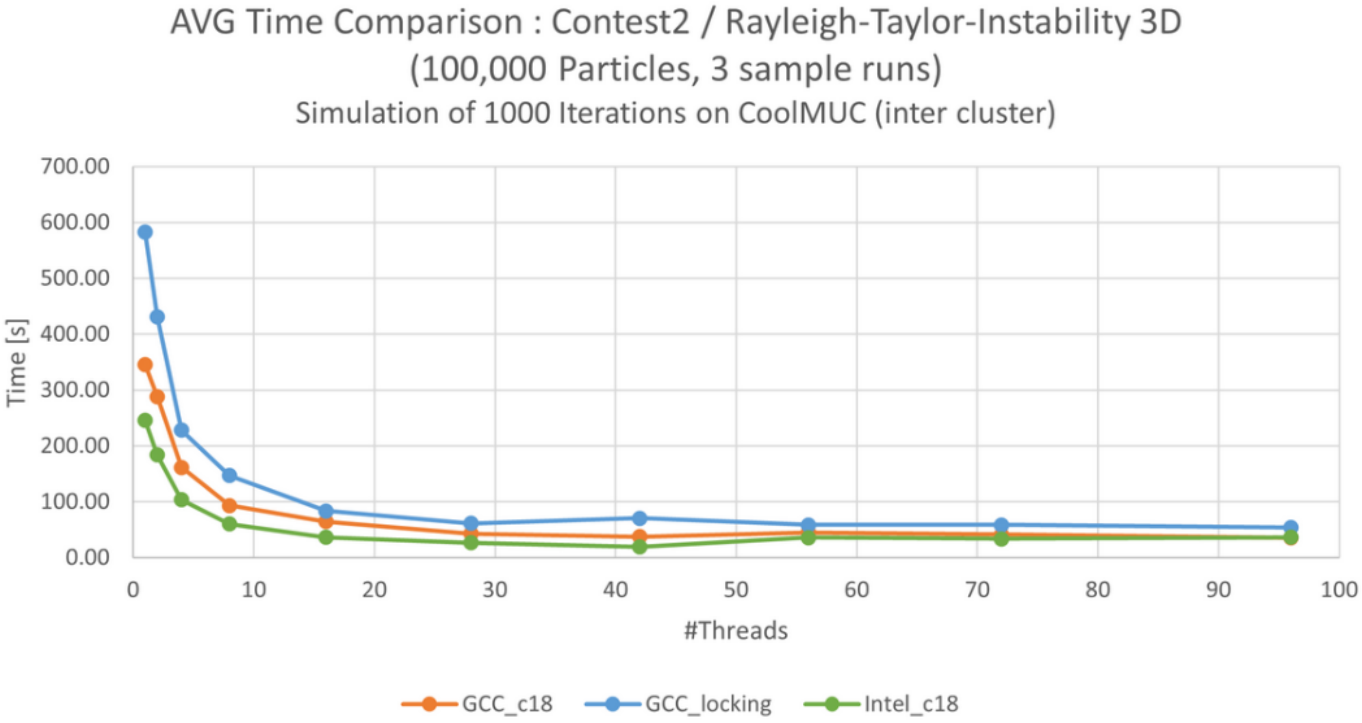
Performance: Speedup



Performance: MUP/s



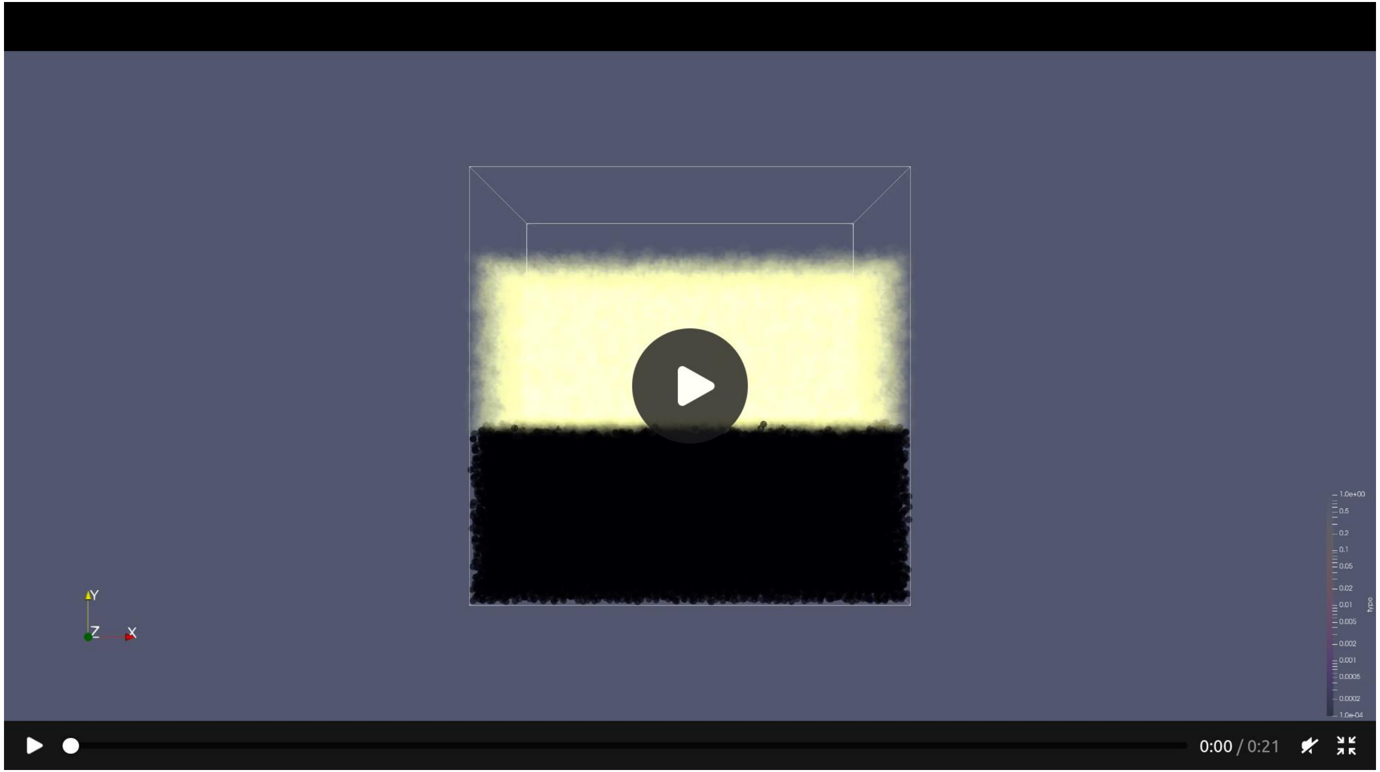
Performance: Time



Contest 2: Rayleigh-Taylor-Instability

- **Remarks:**
  - 42 is the optimal amount of threads
  - Intel compiler has the best performance
- **Data:**
  - **19.25 seconds**
  - **5 193 668 MUP/s**

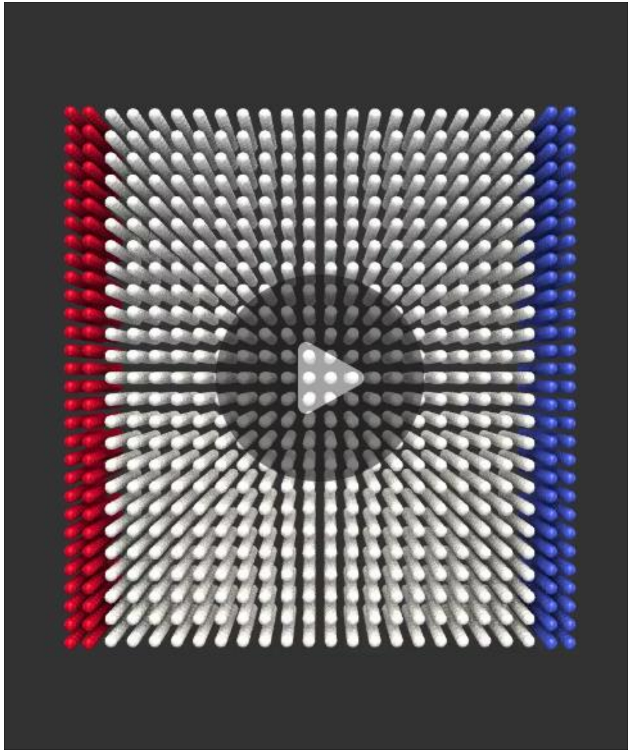
Contest 2: Rayleigh-Taylor-Instability



Nano-scale flow simulation

1

- **New features:**
  1. Fixed flag for particles
  2. New thermostat interceptor
- **Simulations:**
  1. Unhindered flow
  2. Cuboid obstacle
  3. Spherical obstacle
  4. High velocity



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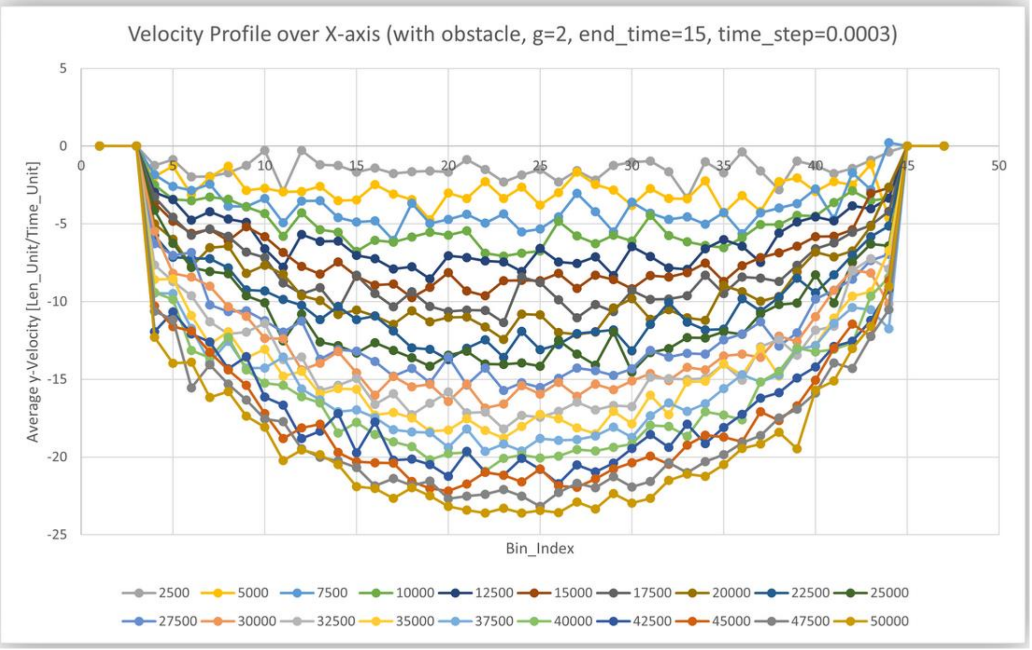

Nano-scale flow simulation

2

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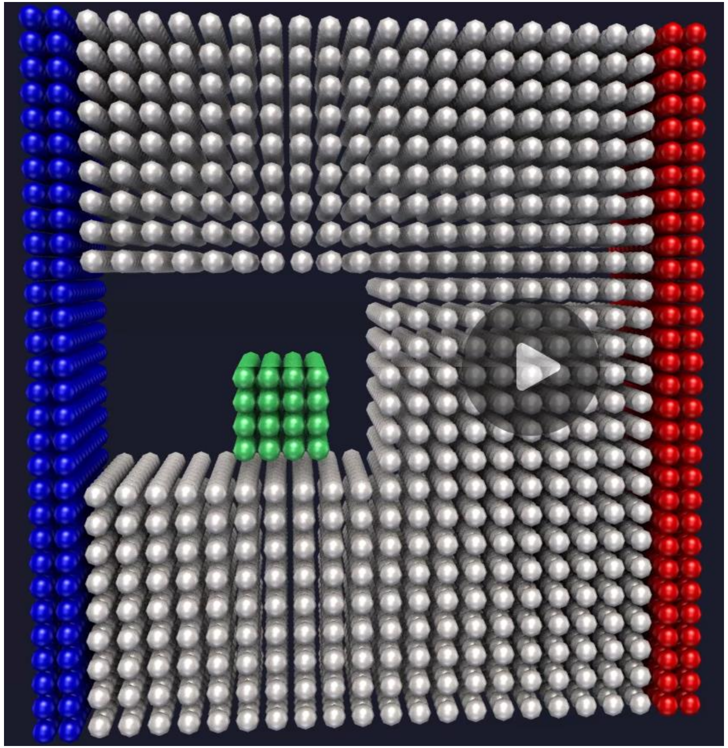
  4. High velocity



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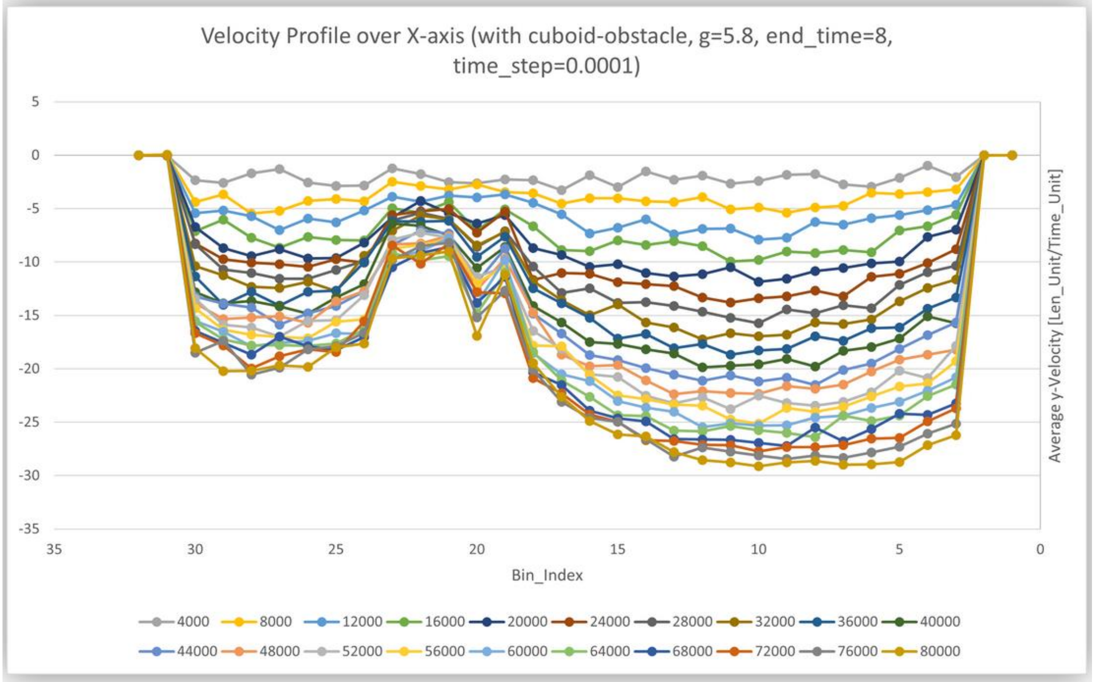

Nano-scale flow simulation

3

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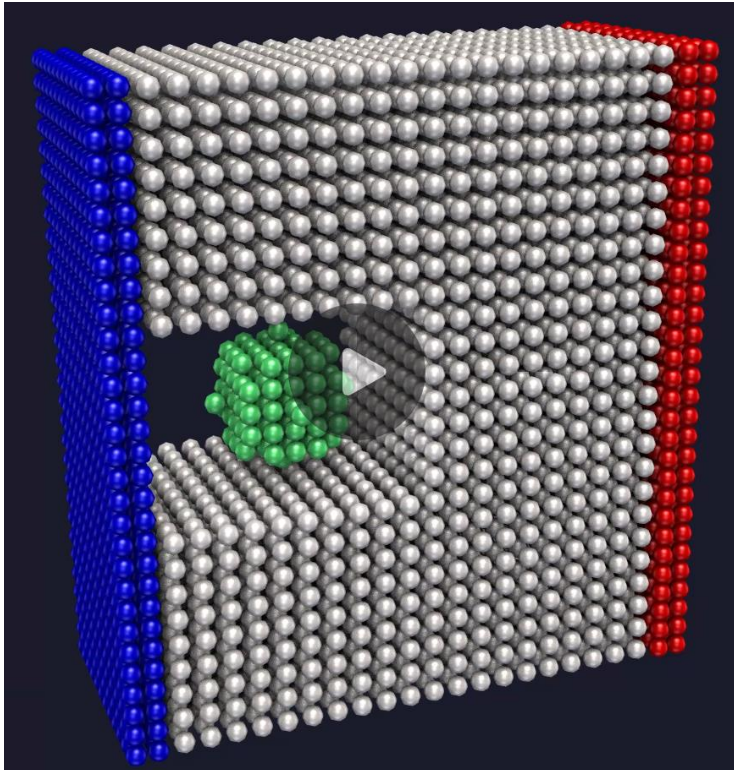

Nano-scale flow simulation

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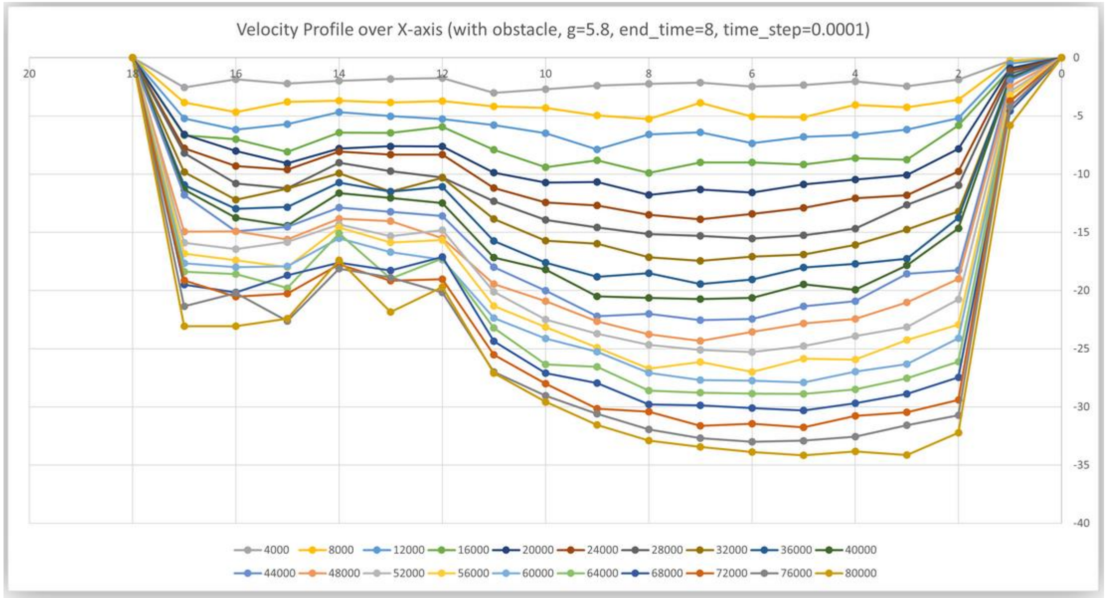

Nano-scale flow simulation

4

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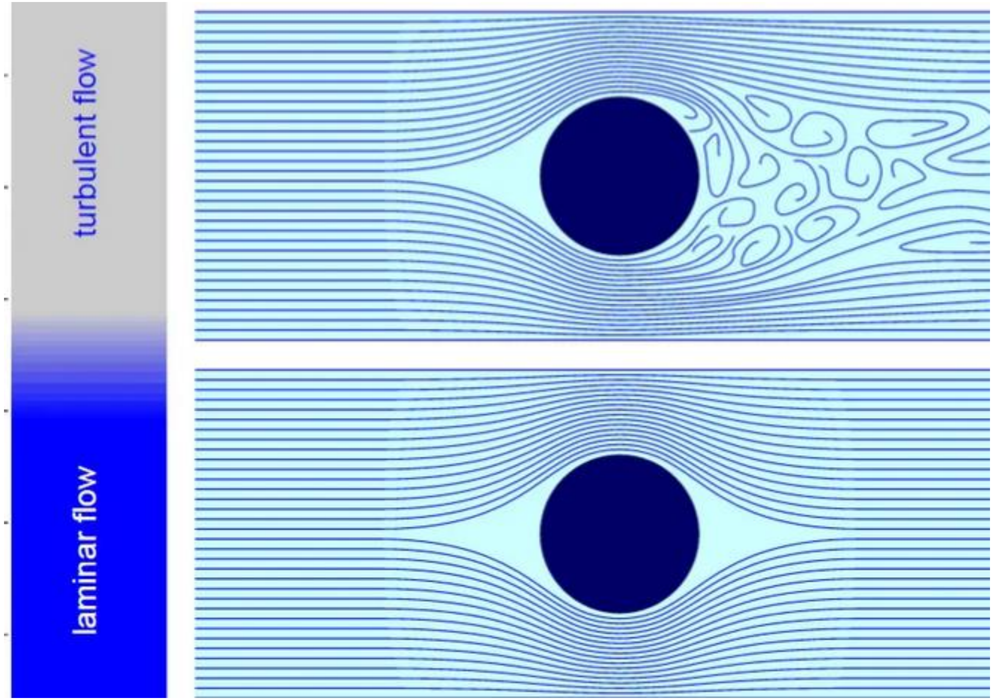
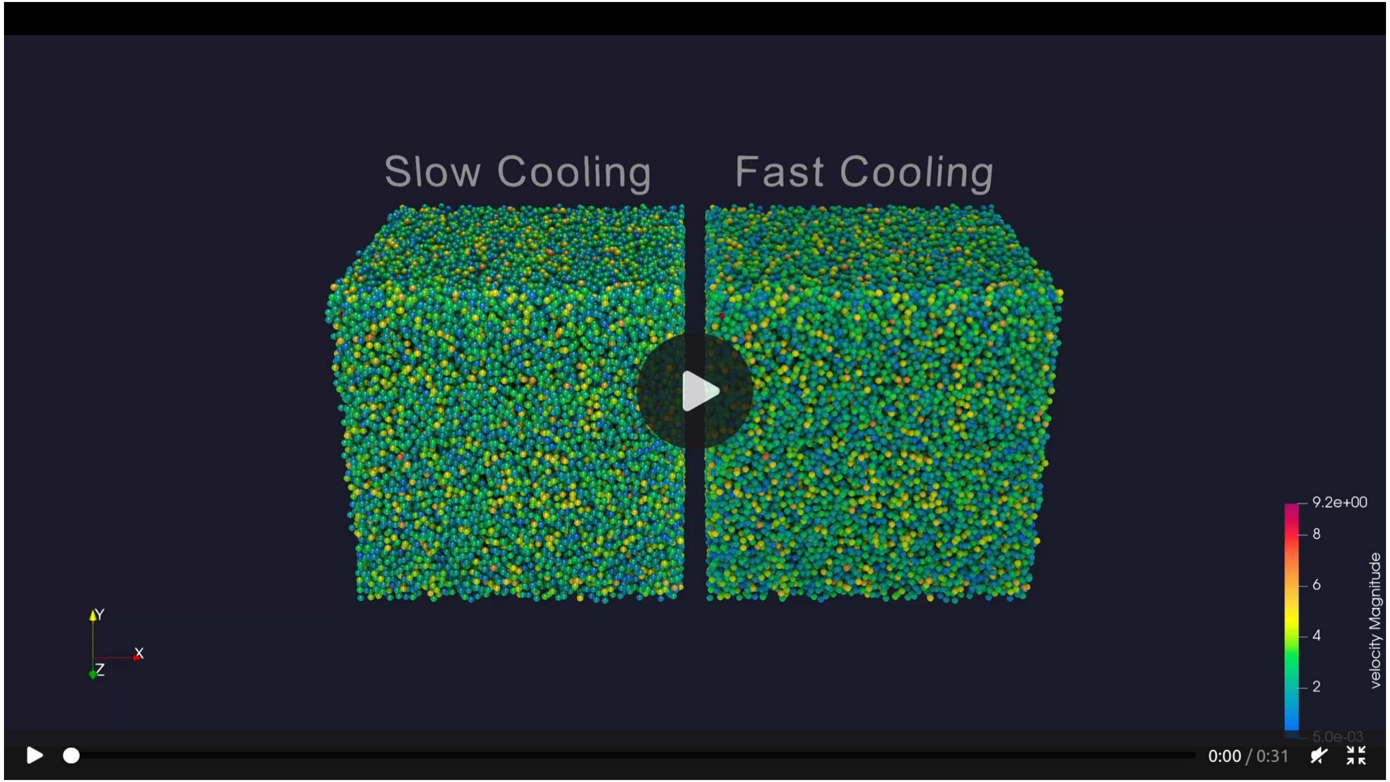


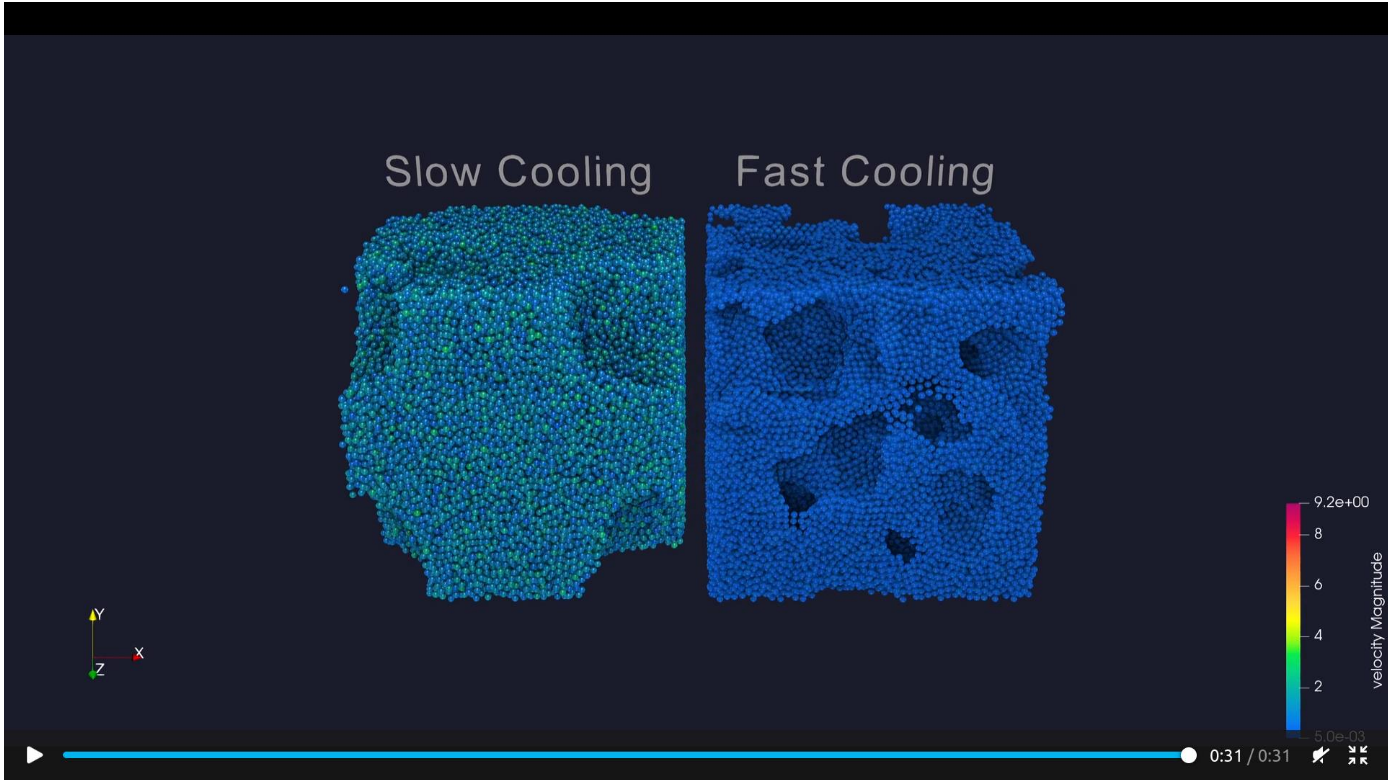
Crystalization of Argon

- **Implementation:**
  - Smoothed Lennard Jones Potential
  - Measurements as Interceptors
- **Qualitative Analysis:**
  - Energy is taken out of the system until the attractive LJ outweighs Temperature
  - Smaller and more holes in supercooled crystal

Crystalization of Argon

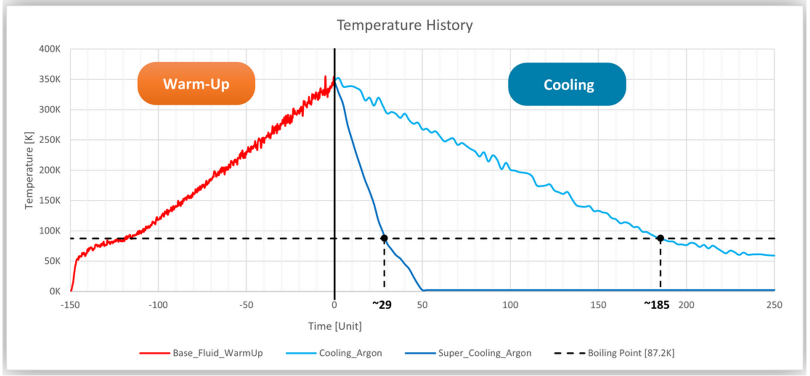


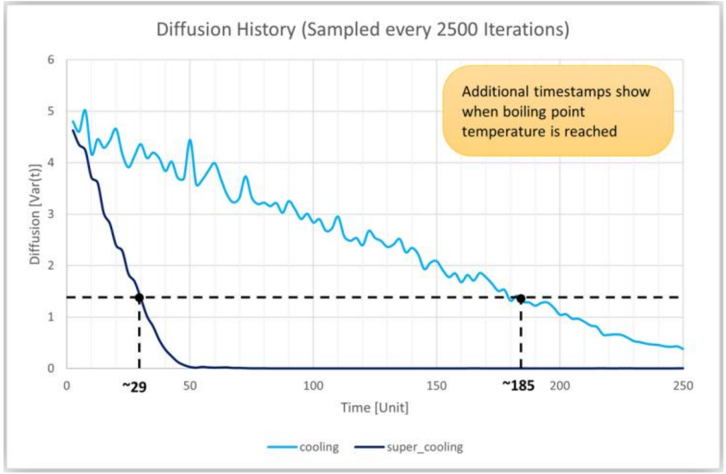
Crystalization of Argon



Crystalization of Argon

- **Quantitative Analysis:**
  - Diffusion & Temperature History
  - Radial Distribution Function
- **Explanation:**
  - Fast nucleation rate
  - Less time to distribute in space





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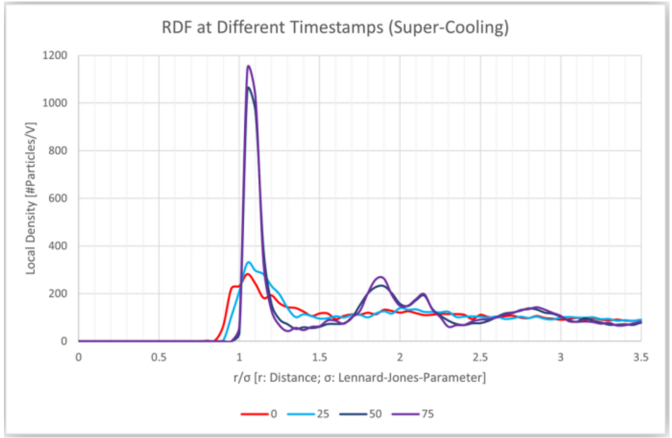

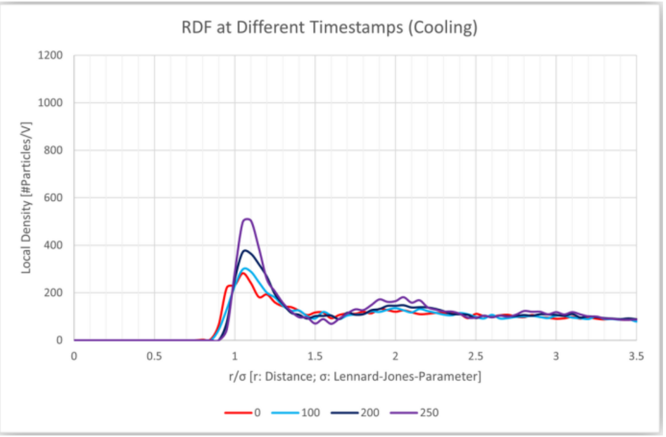

Summary of cool things

- We made a satisfying simulation of rubber cubes
- We read a paper by Prof. Bungatz
- We accelerated the simulation by threading
- We observed unstable chaotic system
- We analysed a particle flow on nano-scale
- We ran hours of argon simulation

References

Waves: https://www.pinterest.de/pin/harmonic-waves-in-architecture-google-search-musicperformance-music-performance-architecture--690247080384012557/
Domain partitioning: https://www.researchgate.net/profile/Fabio-Gratl/publication/357143093_N_Ways_to_Simulate_Short-Range_Particle_Systems_Automated_Algorithm_Selection_with_the_Node-Level_Library_AutoPas/links/649acc9cc41fb852dd355f24/N-Ways-to-Simulate-Short-Range-Particle-Systems-Automated-Algorithm-Selection-with-the-Node-Level-Library-AutoPas.pdf
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