

PSE Molekulardynamik

Sheet 5: Parallelization and Application



Group A: Daniel Schade, Ashutosh Solanki, Robin Cleve

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Simulation of a membrane

- **Implementation**

- Specification of neighbors
- Harmonic force
- Preventing the membrane from self-penetration
- Pulling chosen particles

- **Complications along the way**

Problem: Simulation kept exploding after ca. Iteration 1000!

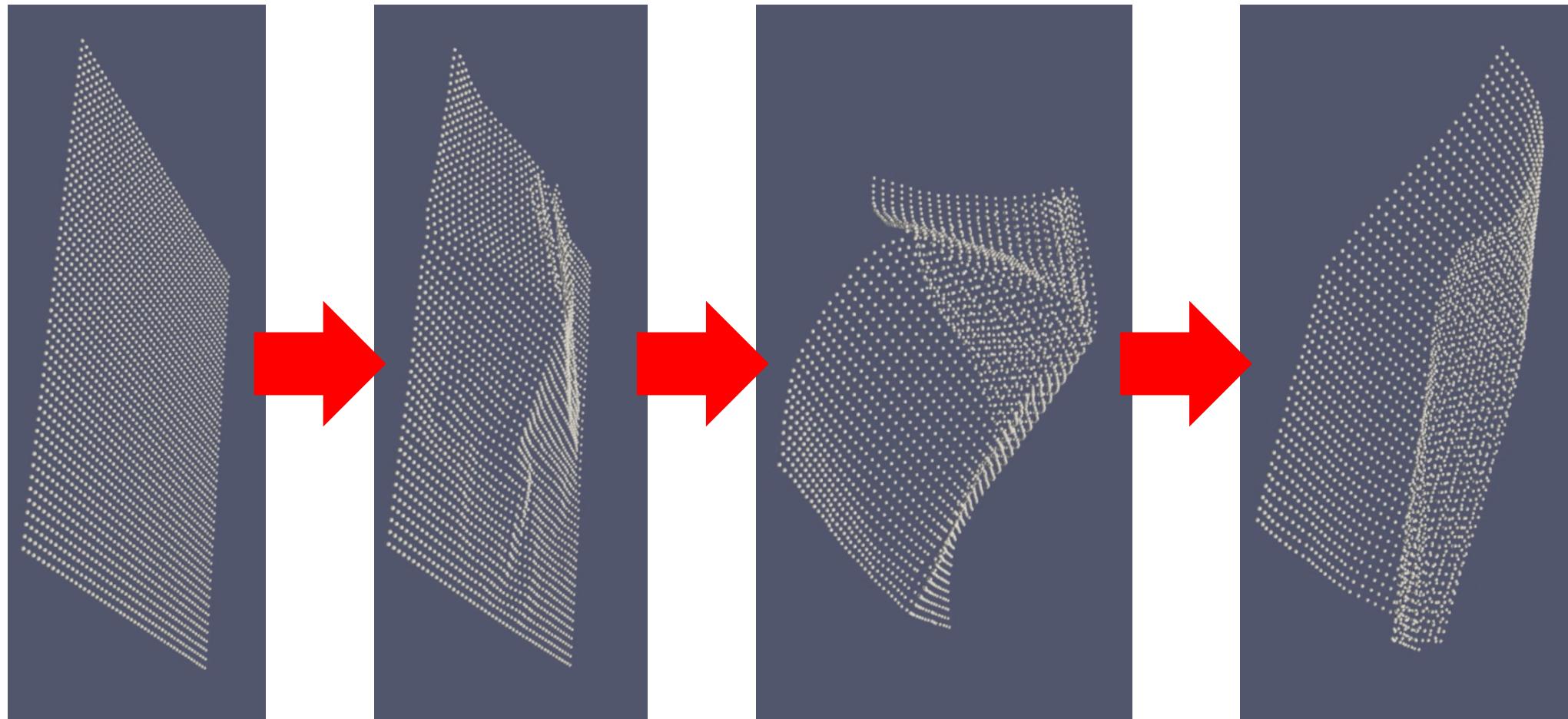
Solution: Wrong Formula for position updates (rooted in the implementation of week 1)

Learning:

- Too confident regarding our code base from previous sheets
- Mistake was too small to influence previous applications (correct test and results so far)
- Kept iterating over implementation of current exercise without looking at old code (for too long)

Simulation of a membrane

Visualization



Parallelization

General

- **Motivation**
 - Change from 2D to 3D causes dramatic increase in runtime
 - **Speed up computation by a constant factor**
- **Setup**
 - Open Mp
 - Easy integration: package search and link to project target in CMakeLists.txt)
 - Program can be used without Open Mp and parallelization
- **What have we parallelized?**
 - Main part force calculation (90% of run time)
 - Velocity and position updates (because it was easy)
 - Processing of boundary conditions (dynamic schedule because of variations between different boundary conditions)

Parallelization

Strategies - avoid race conditions



Iteration of linked cell container, only one thread can have impact on one cell

Strategy 1: Linear

- Linear Iteration over cells x, y, z
- Block each other because of shared neighbor cells

Strategy 2: Skipping

- Skip one cell to prevent two threads from having the same neighbor cells

Strategy 3: Reduction

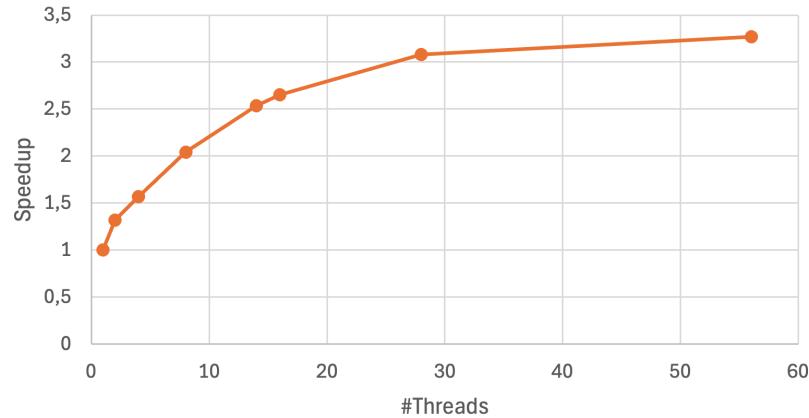
- Very different approach
- every thread has its own force accumulator per molecule
- get reduced afterwards
- **Pro:** no synchronization
- **Con:** massive memory and computation overhead

Parallelization

Strategies – Visualization of speed-up

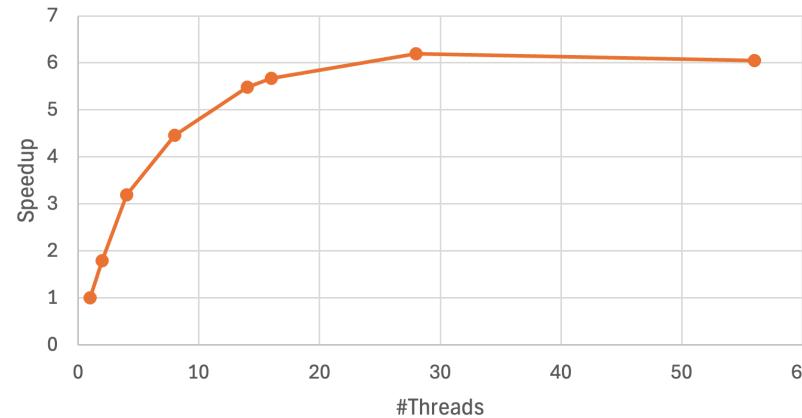
Strategy 1

Performance - Parallelization Strategy Linear



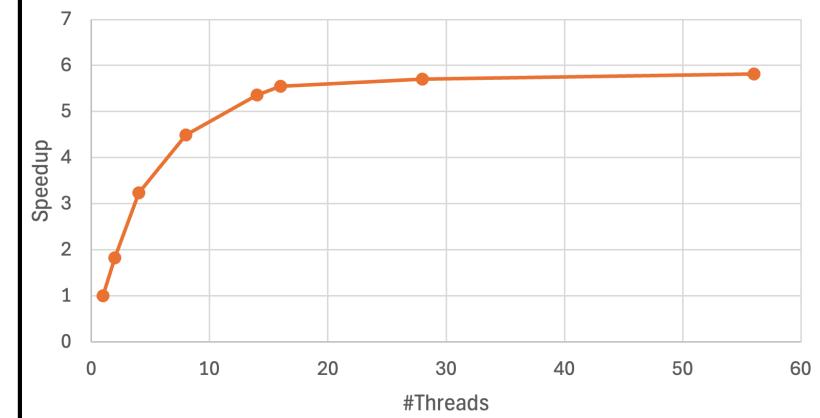
Strategy 2

Performance - Parallelization Strategy Skipping



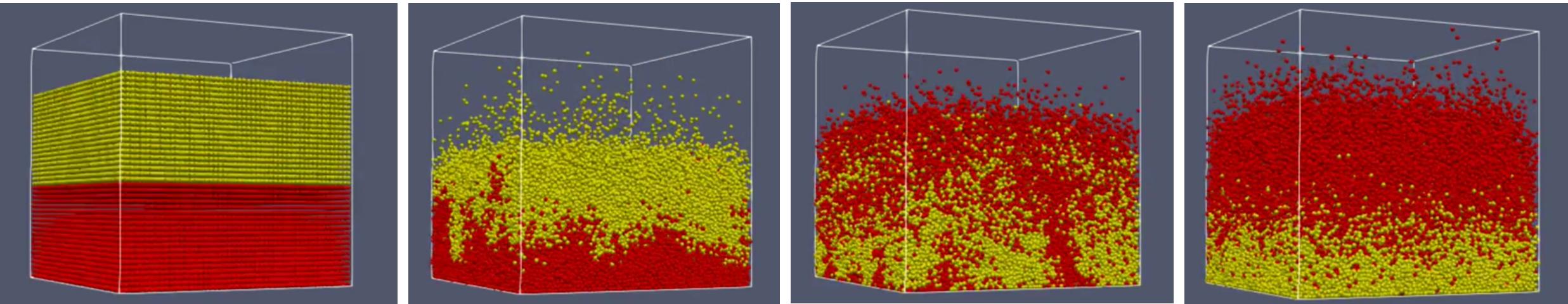
Strategy 3

Performance - Parallelization Strategy Reduction



Rayleigh-Taylor instability in 3D

Over 100.000 molecules, nor further implementation necessary

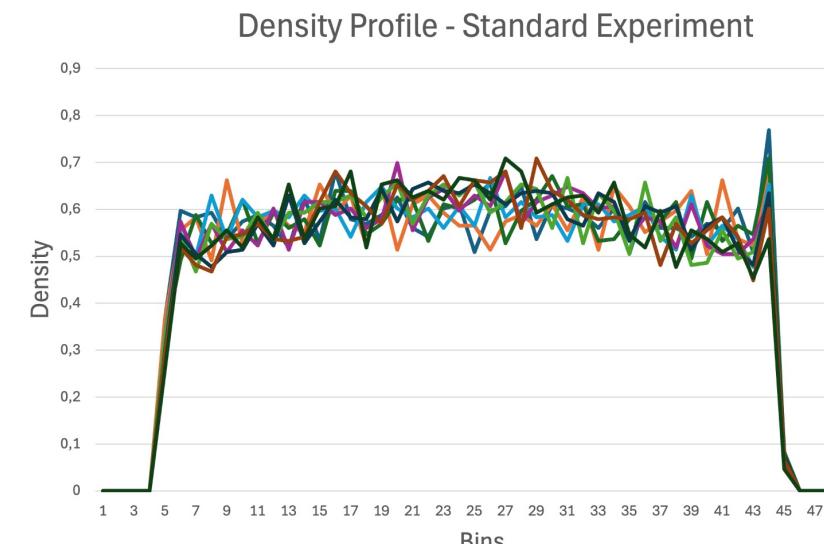
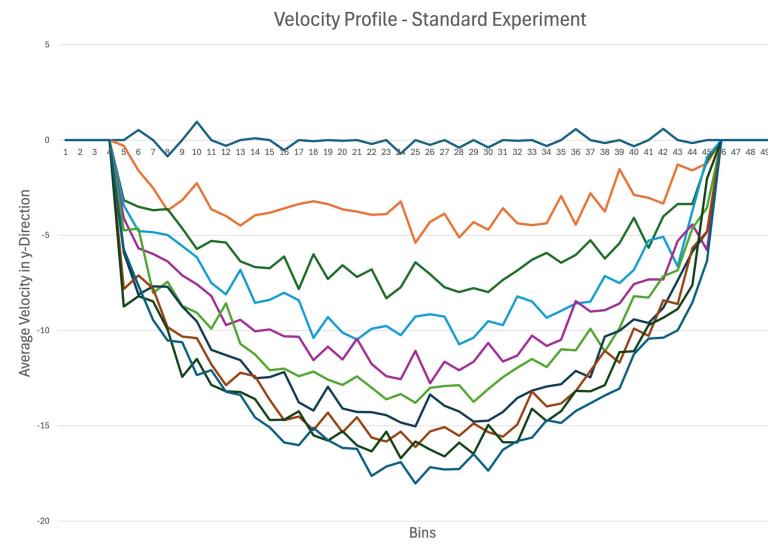


Nano-Scale flow simulation

- **Implementation**

- **Fix the walls:** new bool attribute per particle called “fixed”
- **New thermostat:** ignore velocity of fluid (high temperature -> velocity distribution is heterogeneous)
- Implemented **Profiler** (CSV output)

- **First Experiment**

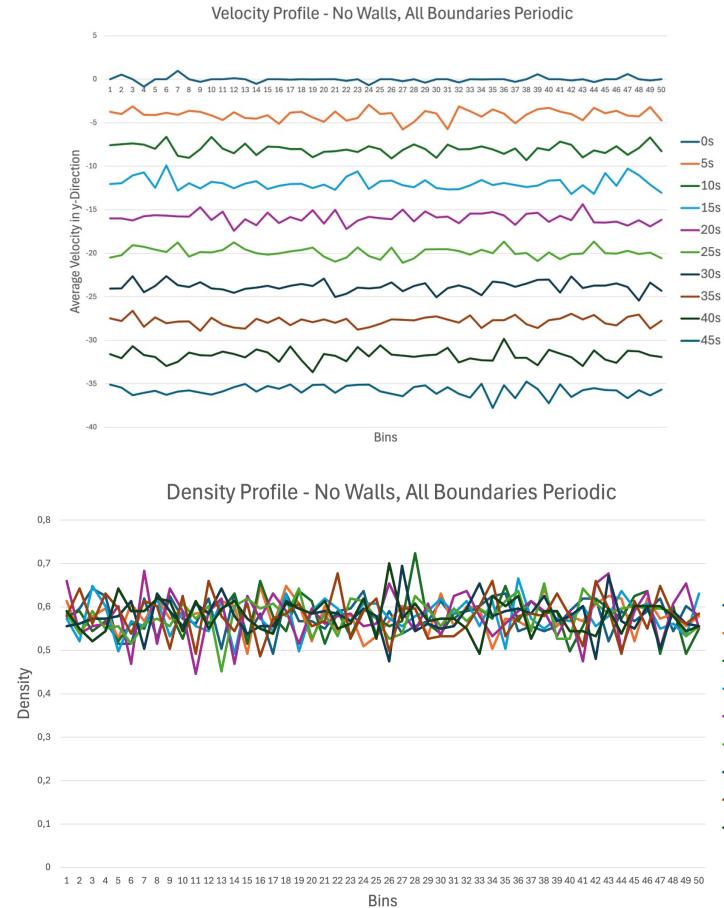


Nano-Scale flow simulation

Increasing sigma



Removing the walls, periodic boundaries



Observing turbulences

