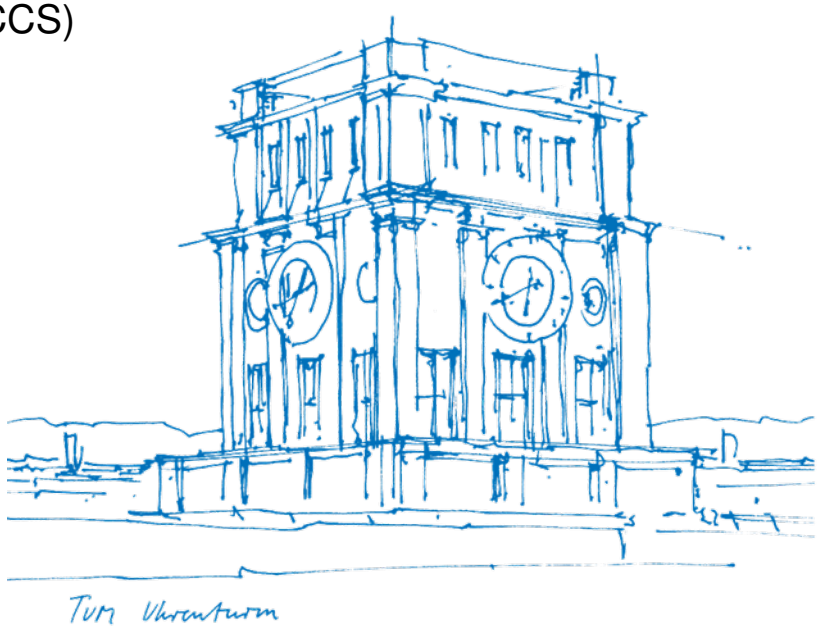
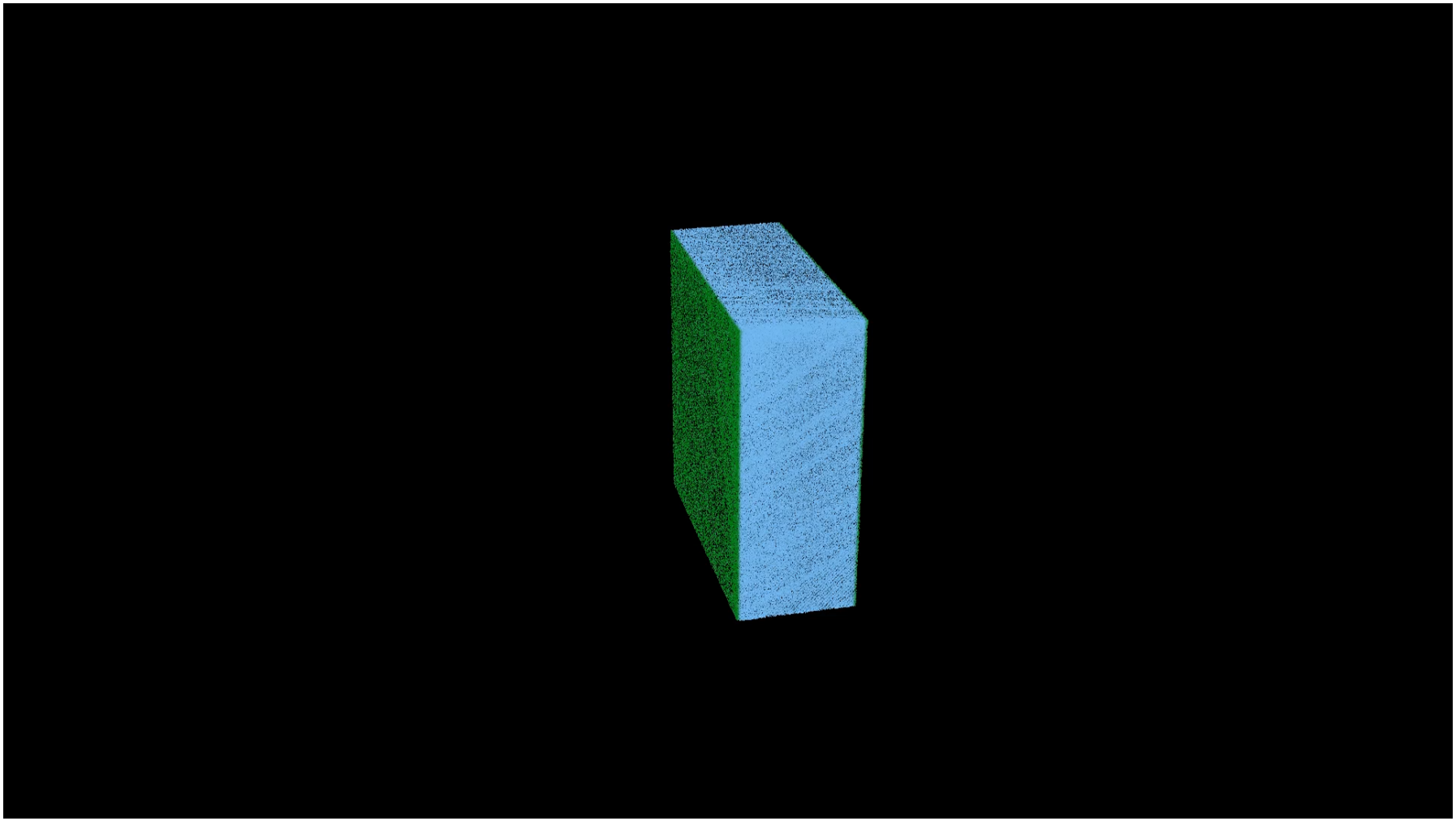
Pimp my Simulation:
Dynamic Algorithm Selection for Particle Simulations

Fabio Gratl, Hans-Joachim Bungartz, Philipp Neumann
Technical University of Munich
Department of Informatics
Chair of Scientific Computing in Computer Science (SCCS)
Leogang, 23.03.2022



Motivation



Molecular Dynamics - Short Range

- Here: small rigid molecules as points without geometry
- Simulation of movement of particles
- Computation of pairwise forces
- Newton's Laws of Motion
- N-Body problem $\Rightarrow O(N^2)$
- Force cut-off $\Rightarrow O(N)$

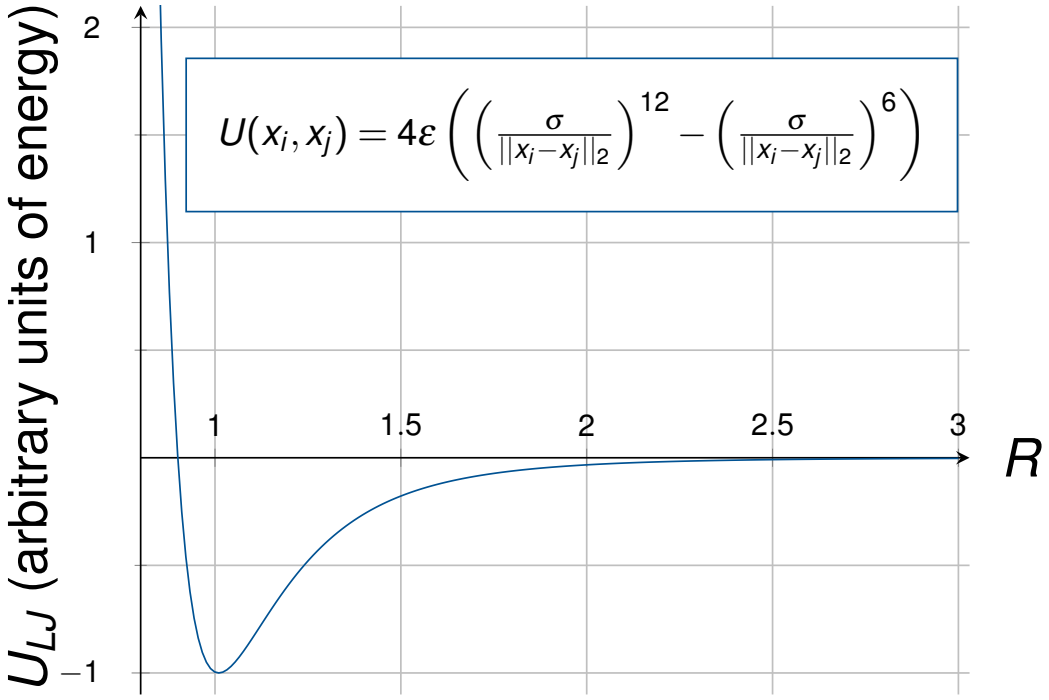
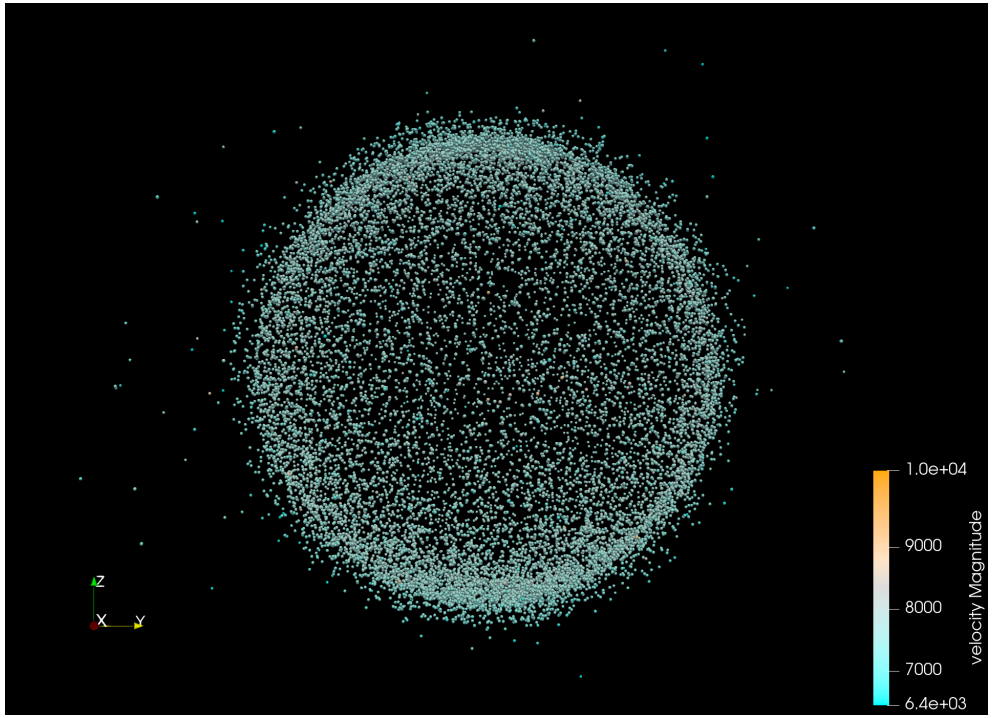


Figure: Lennard Jones Potential for $\varepsilon = 1$ and $\sigma = 0.9$

Challenges

- Total number of particles
- Particle density
- (In-)Homogeneity
- Systems changing over time
- Many possible algorithms
- Arbitrary simulation types:
  MD, SPH, DEM, ...
- Overall goal:
  Minimize time to solution!

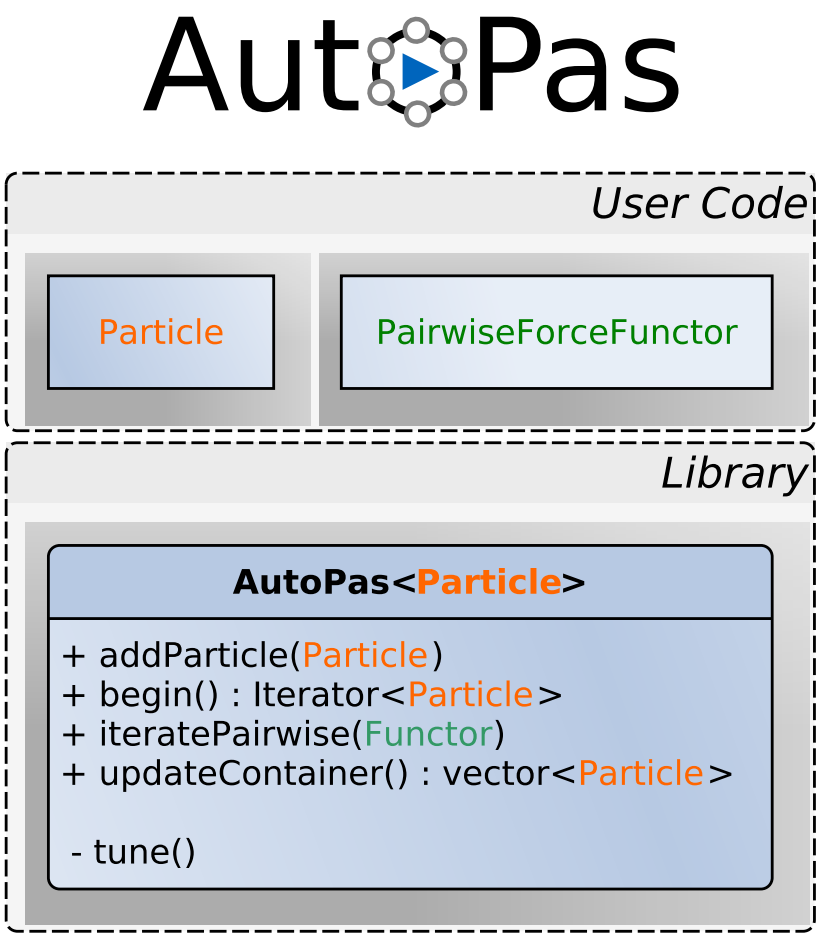


Introducing AutoPas

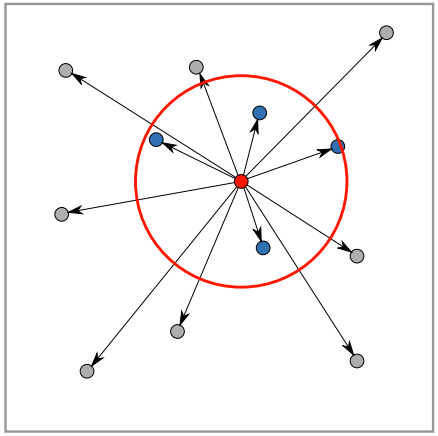
- Node-Level `C++17` library
- Black-box particle container
- Facade-like software pattern
- User defines:
  - Properties of particles
  - Force for pairwise interaction
- AutoPas provides
  - Containers, Traversals, Data Layouts, ...
  - Dynamic Tuning at run-time

⇒ General base for N-Body simulations

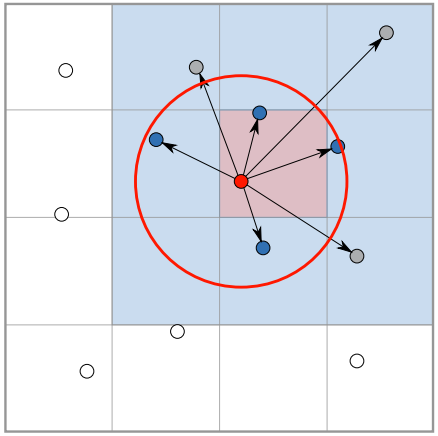
https://autopas.github.io/



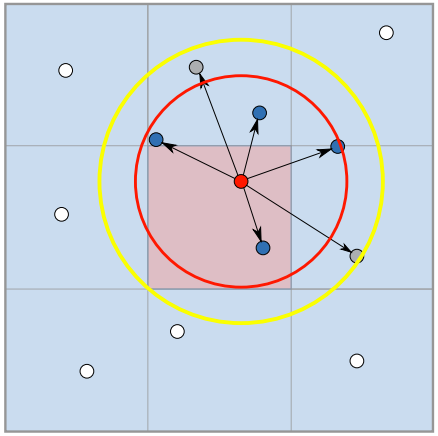
Algorithmic Choices



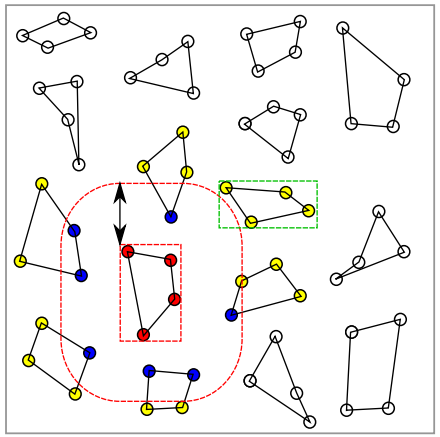
Direct Sum



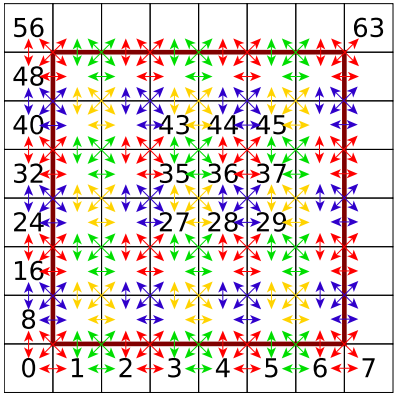
Linked Cells



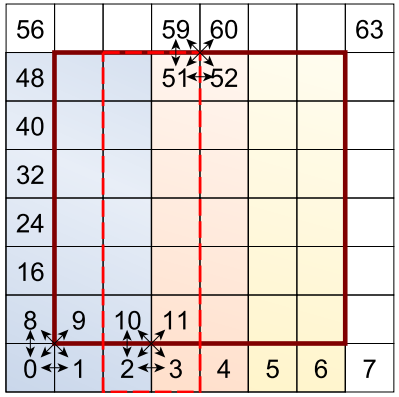
Verlet Lists



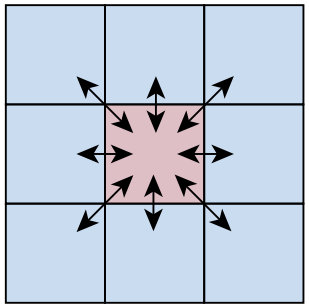
Verlet Cluster Lists



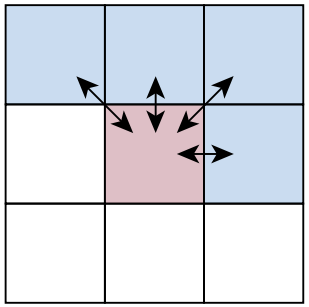
Coloring



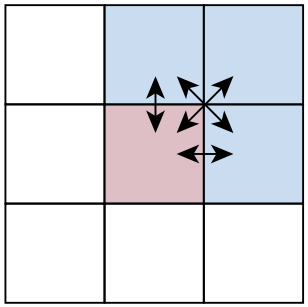
Slicing



C01



C18

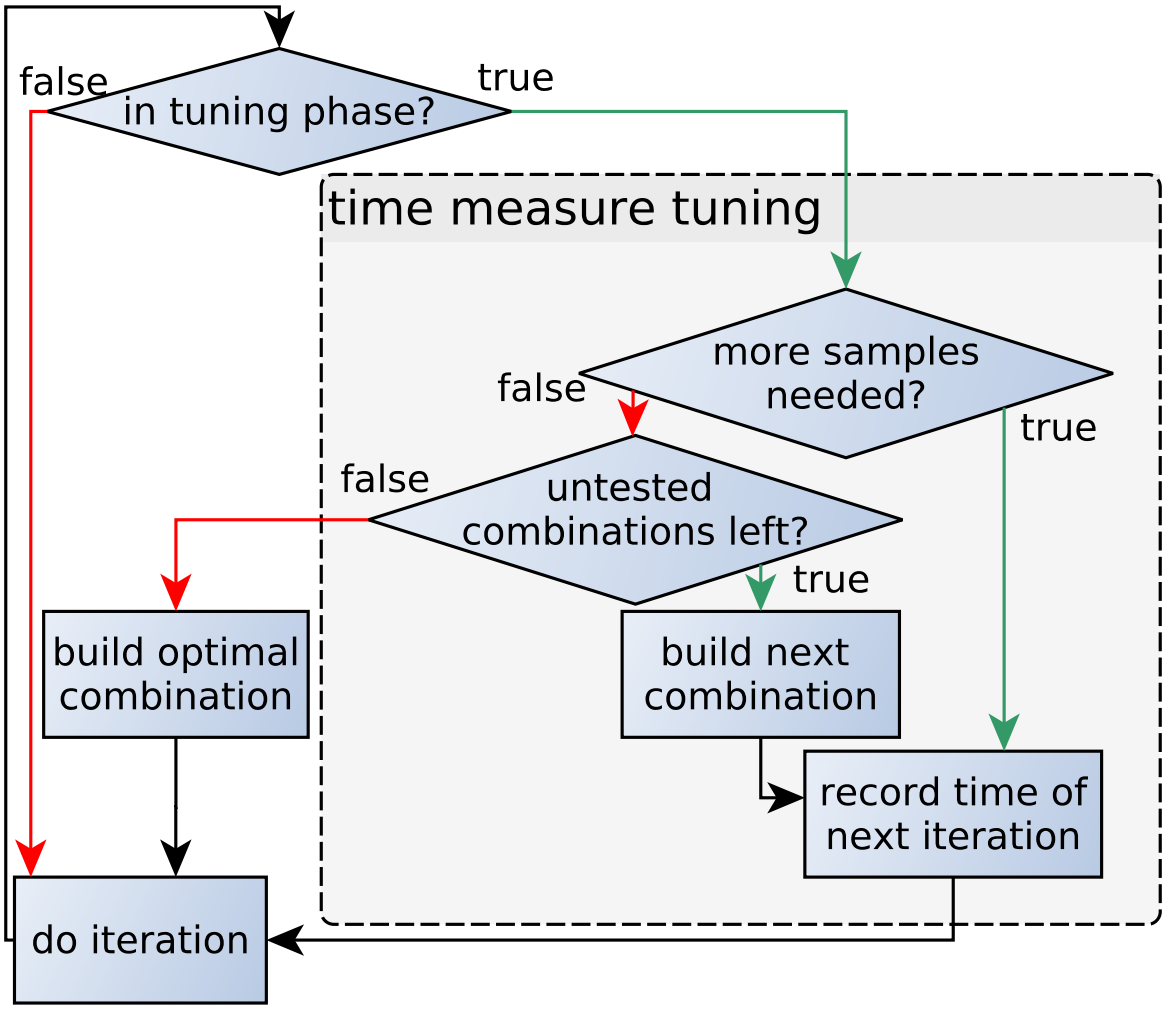


C08

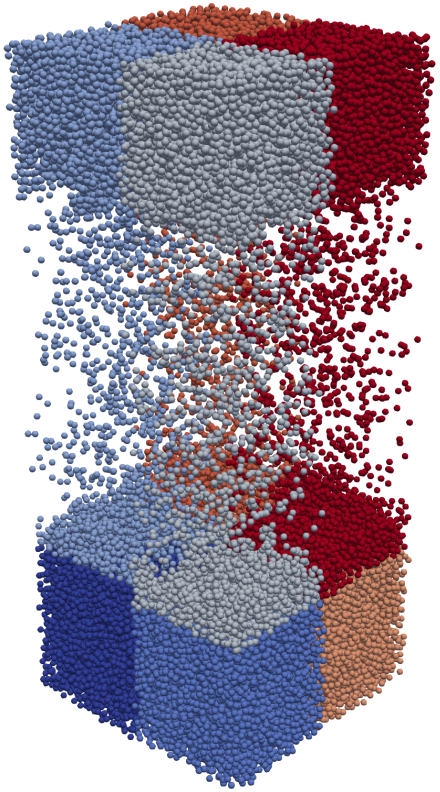
Stencils

Tuning Cycle

- Common interfaces for containers, traversals, etc
- Repeated periodically
- User can restrict search space

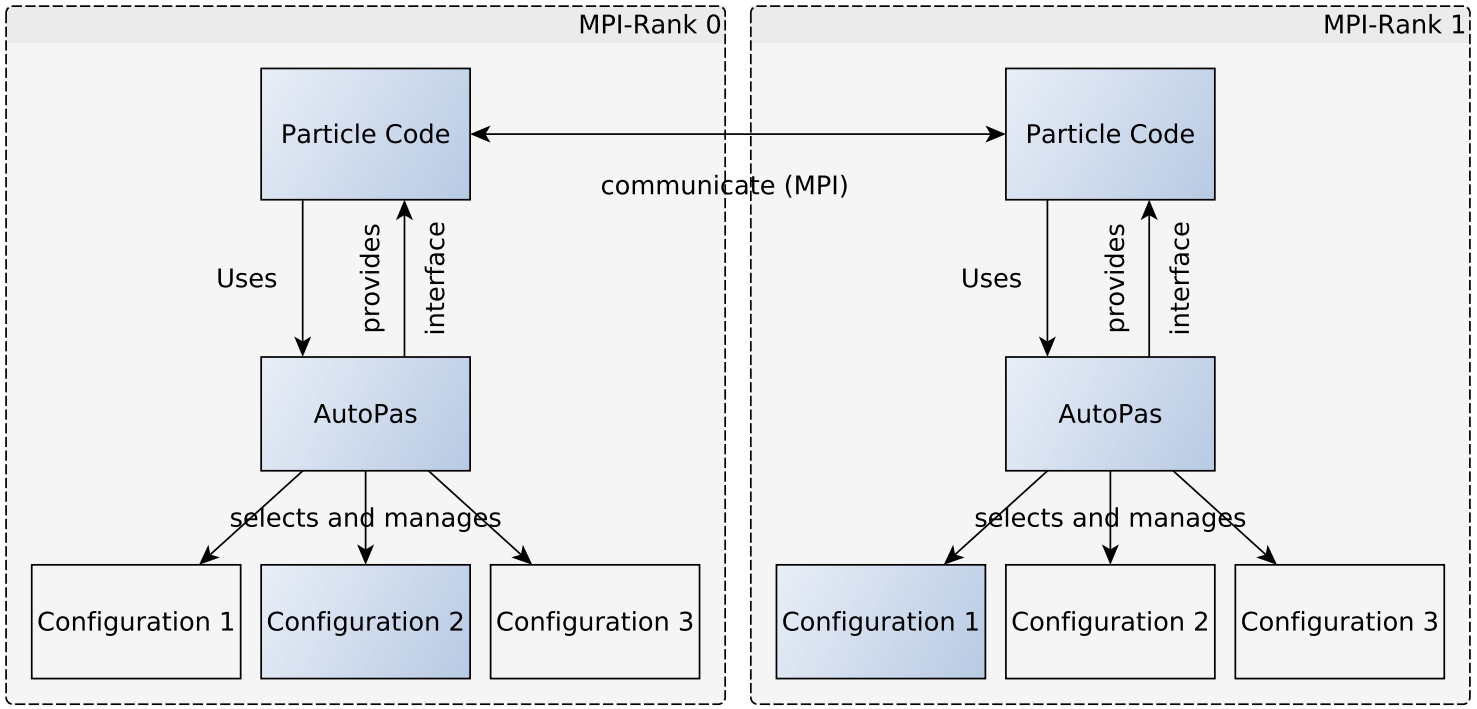


Predictive Tuning



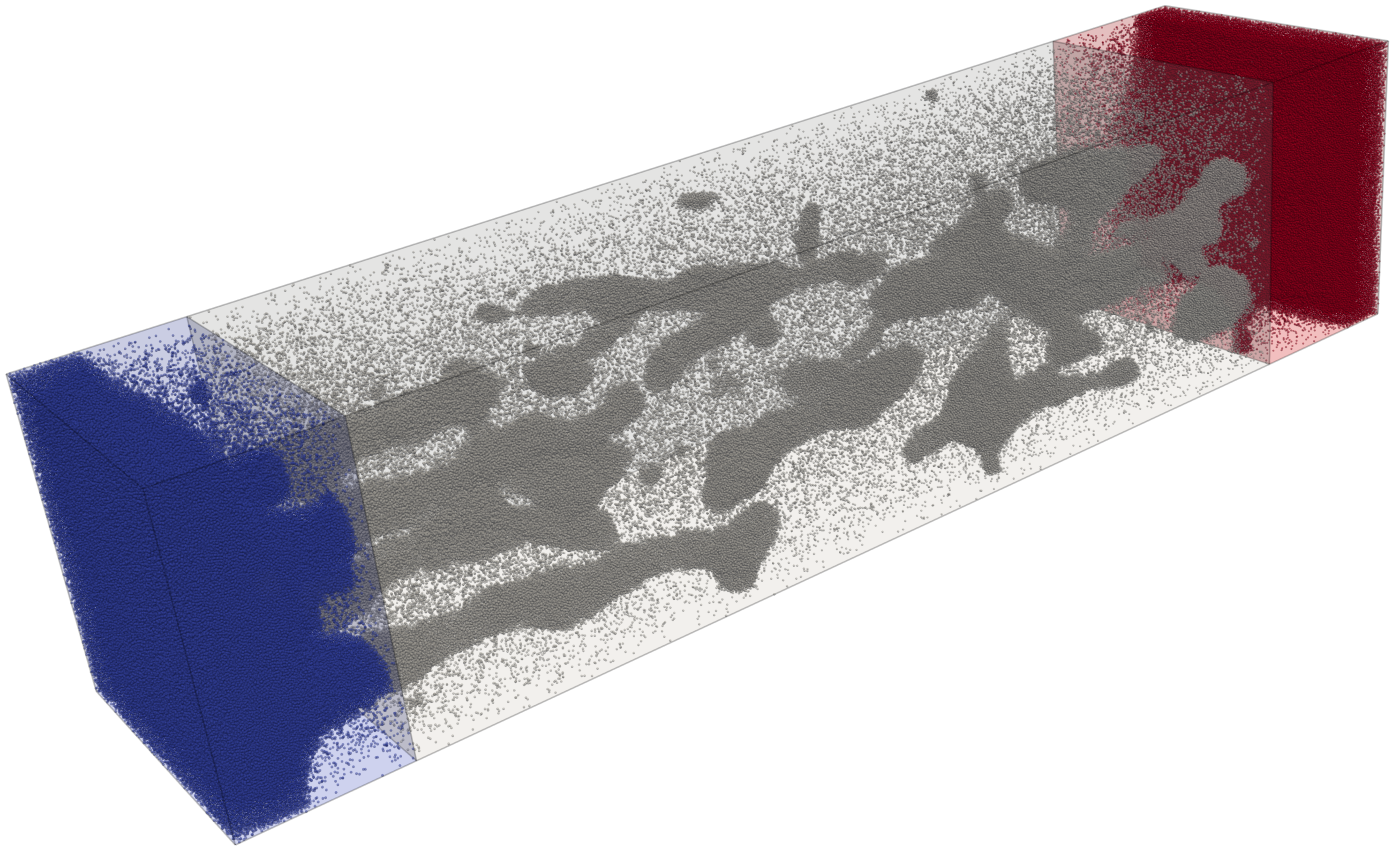
- Testing only promising configurations reduces runtime

AutoPas in MPI parallel Software

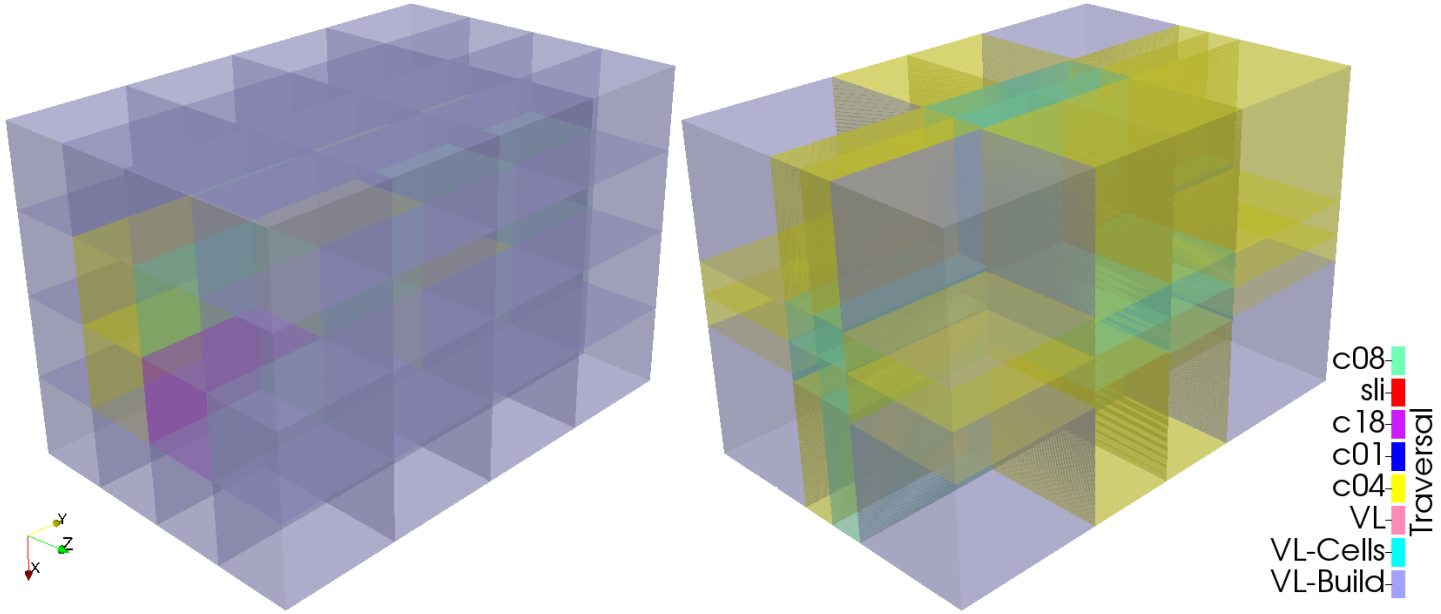


- One AutoPas instance per Rank.
- Independent tuning!
- Interfaces independent of algorithms.
- AutoPas acts as black-box container.

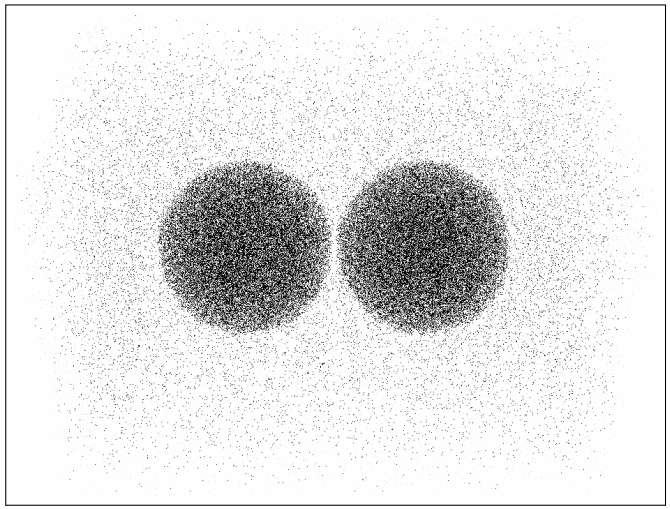
ls1 mardyn + AutoPas $\Rightarrow$ MPI + Tuning



Speedups from Dynamic Tuning

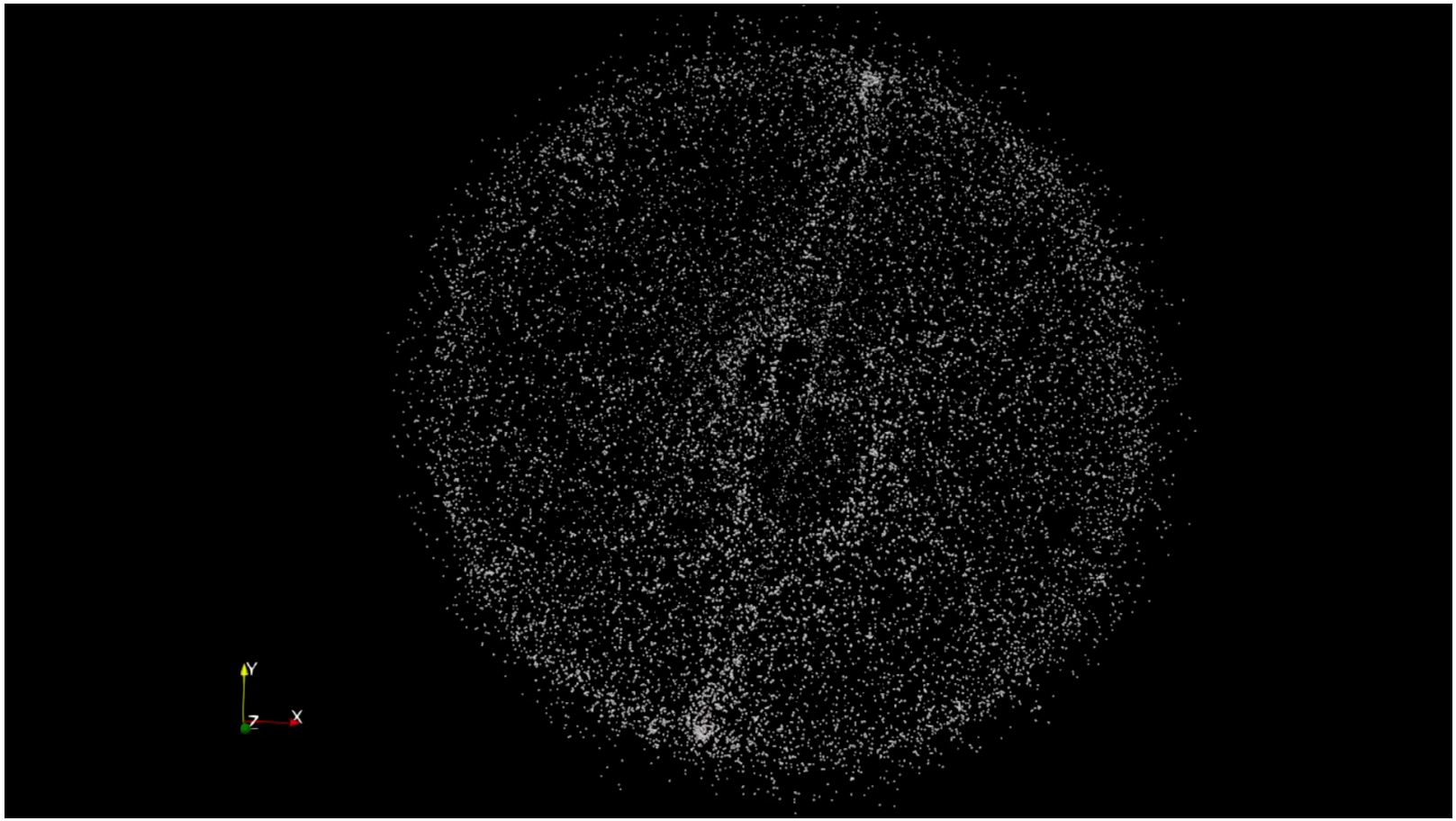


- 64 Ranks; 3M particles
- Auto-Tuning + Diffusive Loadbalancing
- Speed-up about 50% vs vanilla ls1



Seckler, S., Gratl, F., Heinen, M., Vrabec, J., Bungartz, H. J., & Neumann, P. (2021). AutoPas in ls1 mardyn: Massively parallel particle simulations with node-level auto-tuning. Journal of Computational Science, 50, 101296.

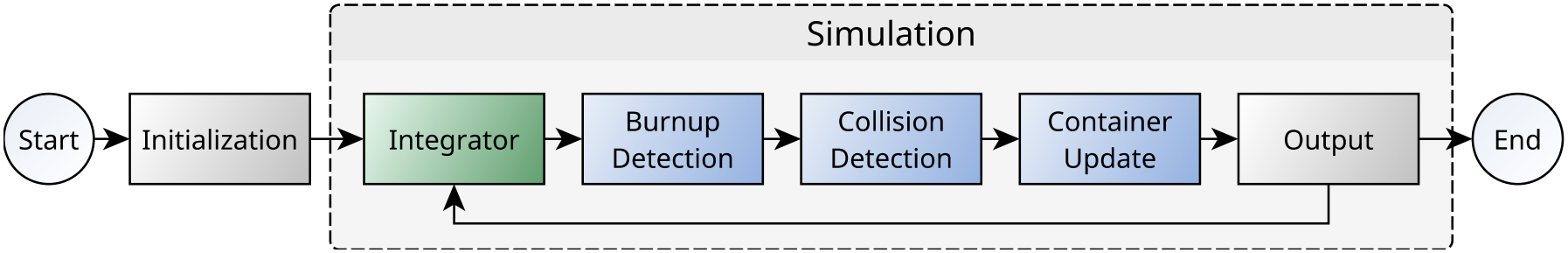
Different Context: Space Debris Simulation



- Cooperation TUM $\Leftrightarrow$ ESA ACT
- Deterministic Collision Tracking
- Simulate Satellites as Particles
- Pairwise Interaction = Collision

LADDS - Overview

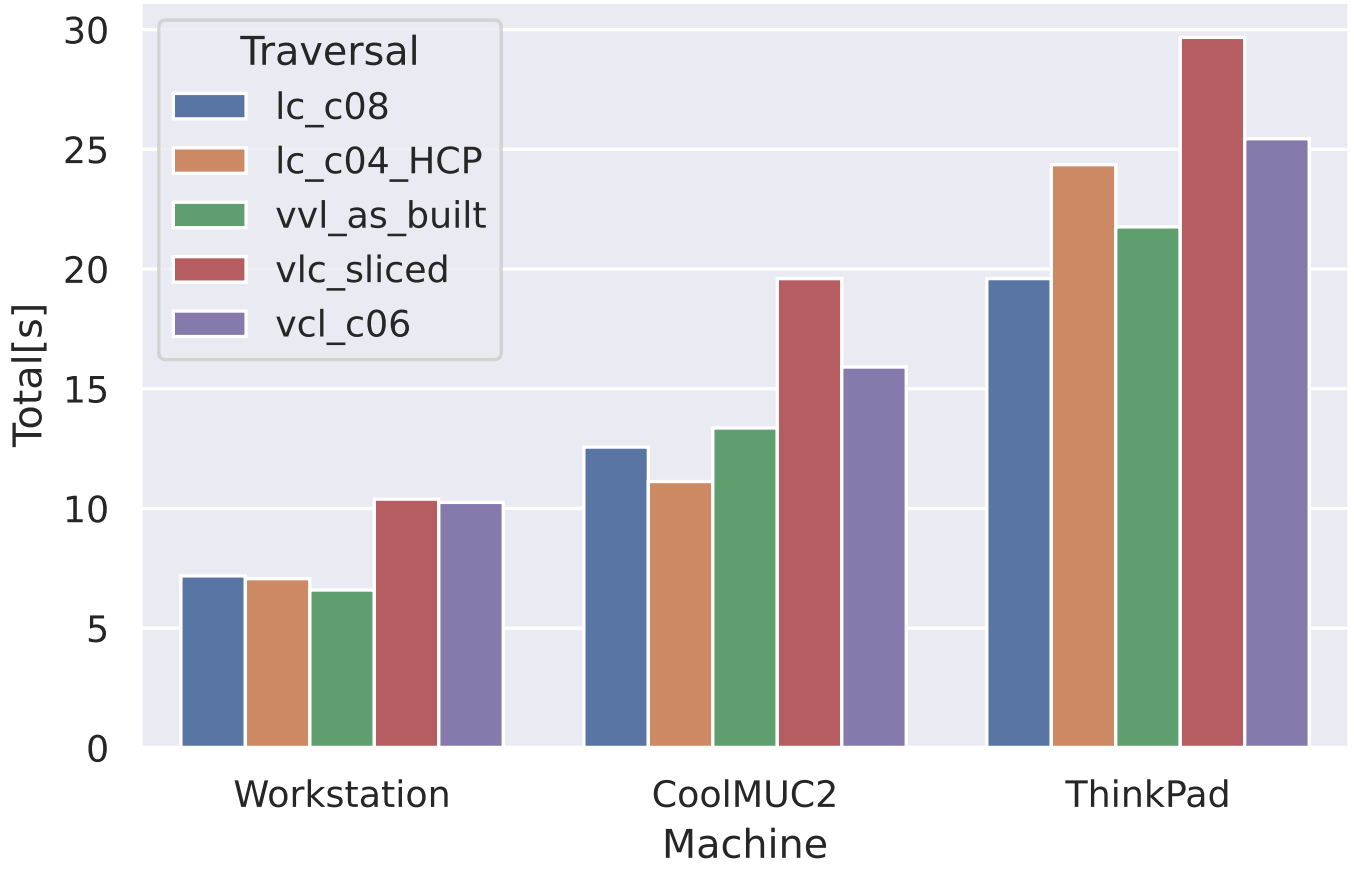
- Modular Design
  - AutoPas as main Particle Container
  - Integrator
  - Break-up Model
- Most of the algorithmic burden on AutoPas
  $\Rightarrow$ Great development accelerator!



Gómez, P., Gratl, F., Bösing, O., & Izzo, D. (2022).

Deterministic Conjunction Tracking in Long-term Space Debris Simulations. IAA-ICSSA-22-0000.

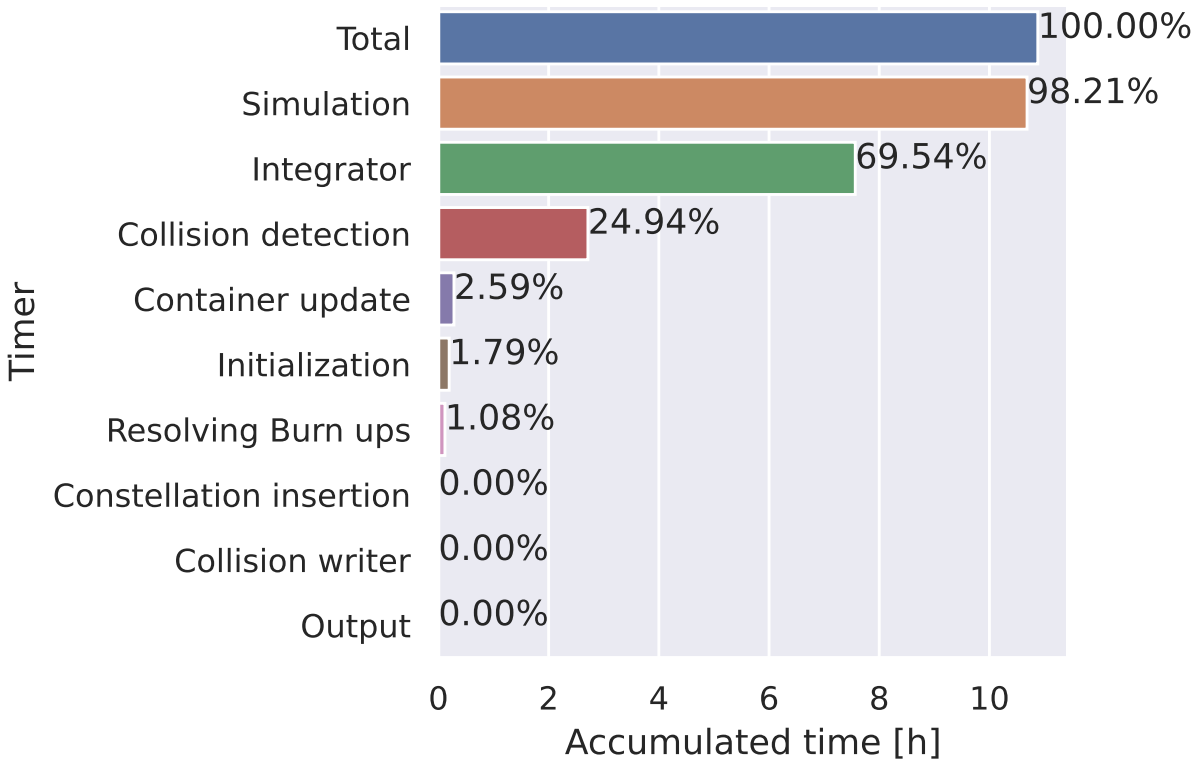
LADDS - Find the Optimal Algorithm



1000 iterations with $>$16k particles

LADDS - Runtime Distribution

- Currently Pairwise Iteration not dominant part
- Will change with more particles
- Even more scaling via MPI



Summary

- AutoPas enables automated algorithm selection on node level.
  - Independent tuning of all MPI ranks.
  - Optimal algorithm choices also for non-expert users.
- Dynamic algorithm selection has potential to significantly speed-up simulations.
- Black Box particle container facilitates development of new applications.
  - Adapts to changing requirements.
  - No expert knowledge needed.