AutoPas & *ls1 mardyn*: Enabling Auto-Tuning in MPI+X Load-Balanced Molecular Dynamics Simulations

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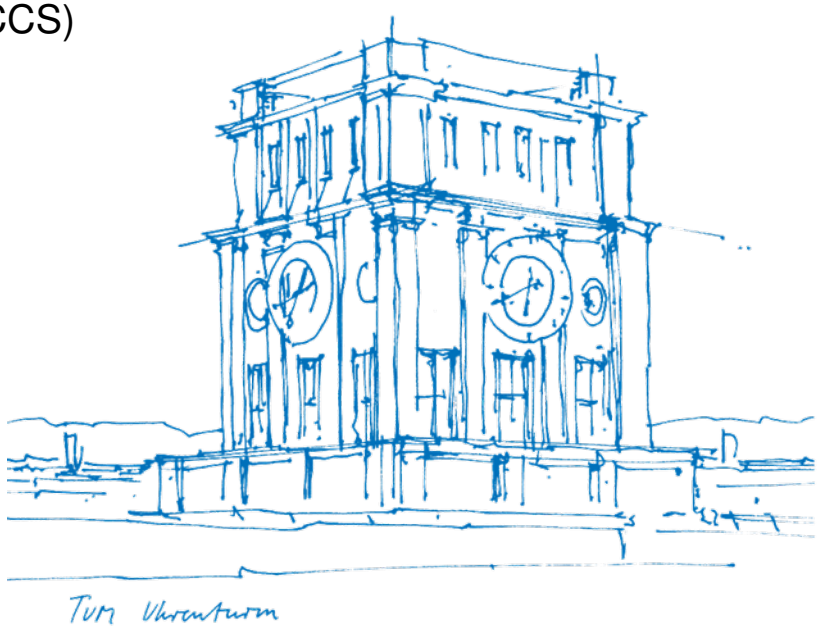

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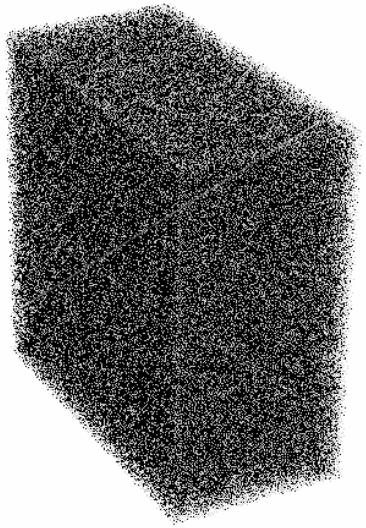
Motivation



Outline

AutoPas

ls1 mardyn

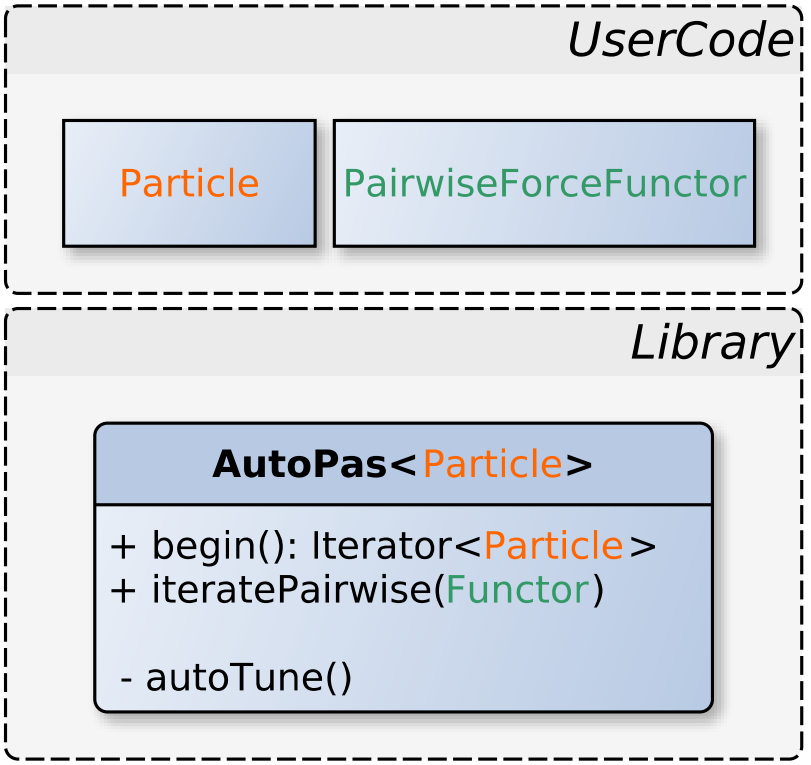
Experimental Results

AutoPas

AutoPas: Overview

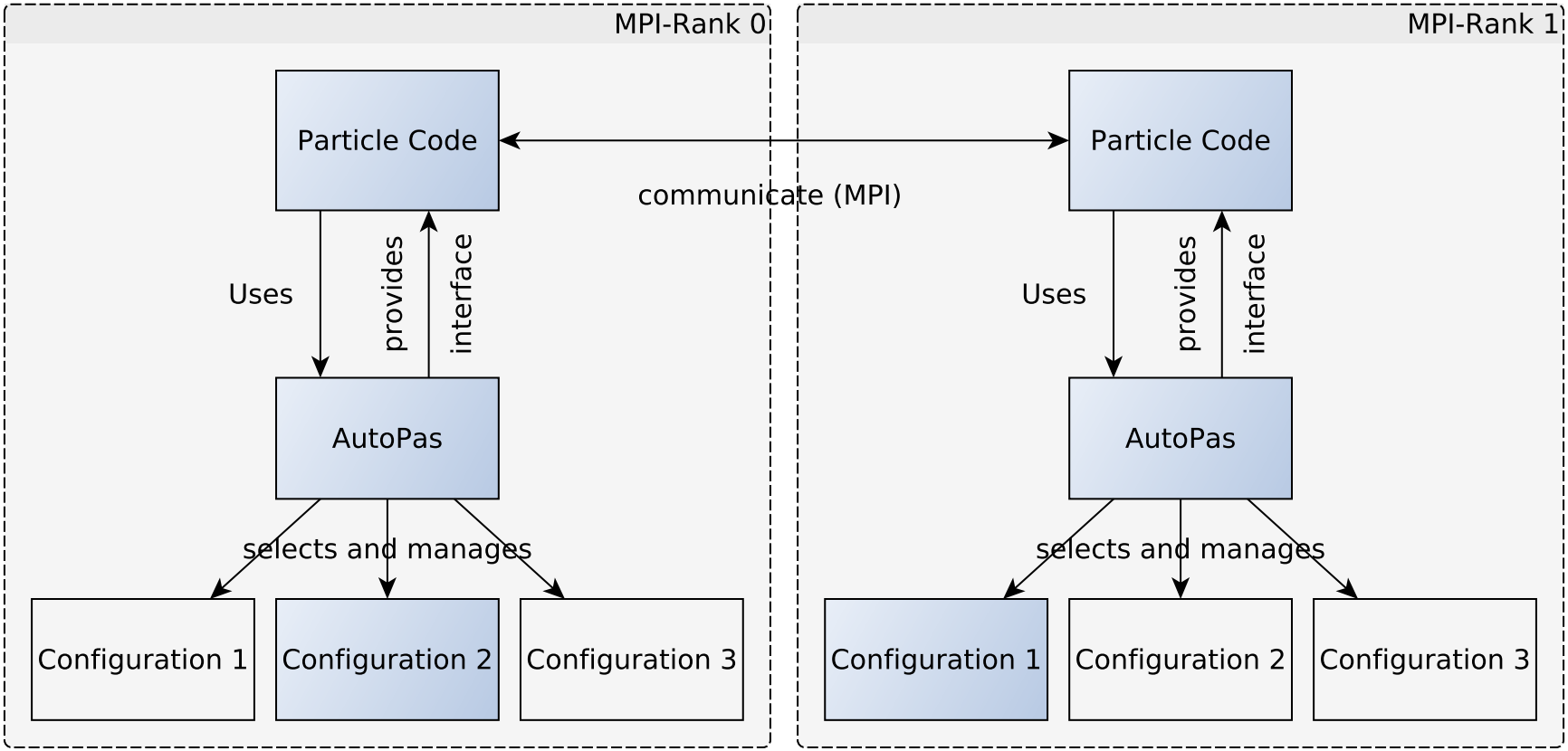
- Node-Level C++ library
- User defines:
  - Properties of particles
  - Force for pairwise interaction
- AutoPas provides:
  - Containers, Traversals, Data Layouts, ...
  - Dynamic Tuning at run-time
- Black Box container

$\Rightarrow$ General base for *N*-Body simulations



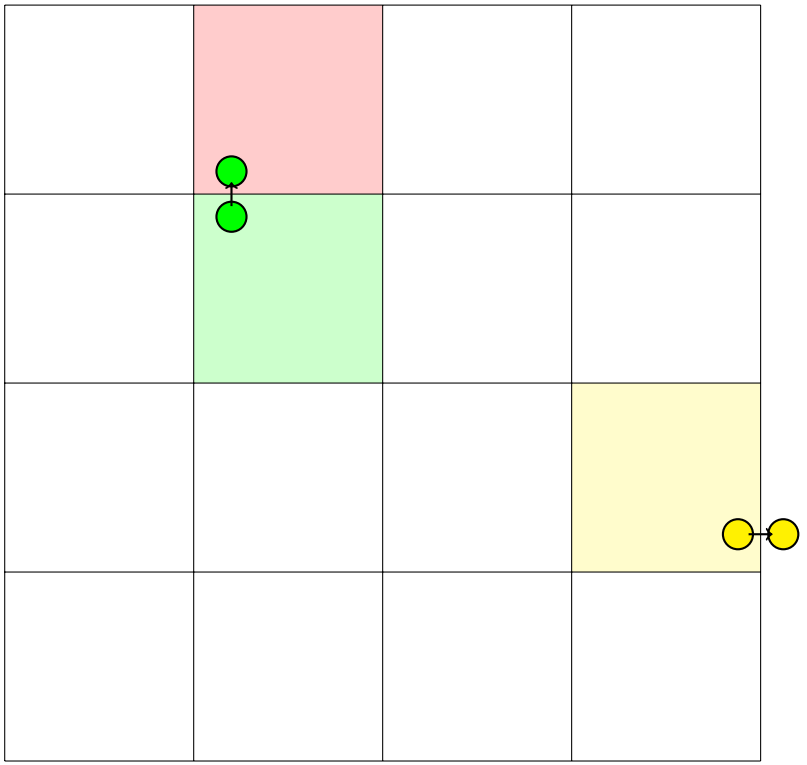
https://github.com/AutoPas/AutoPas

AutoPas Interface



AutoPas Interface

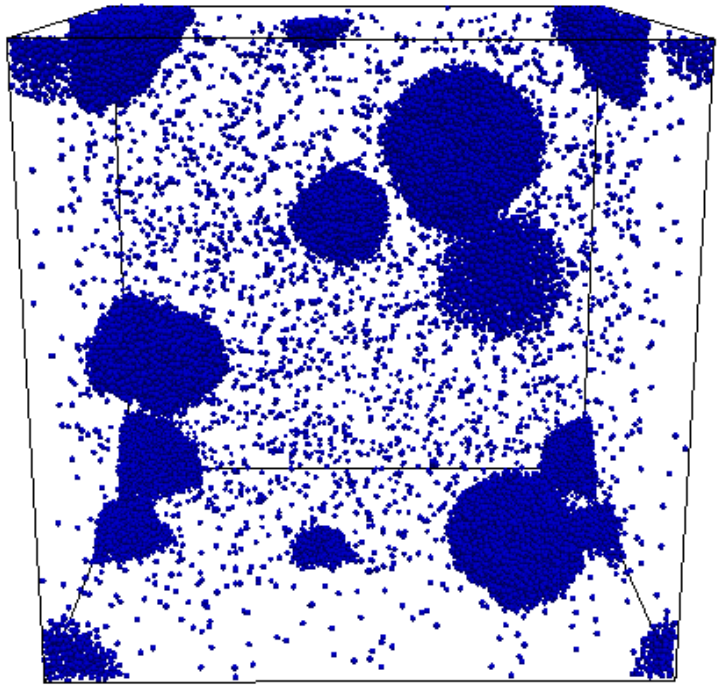
- One common interface for the AutoPas class and all its containers.
- Interface is compatible to neighbor list approaches:
  - Update container structure only every N time steps (reuse of neighbor lists).
  - Move particles between ranks only every N time steps.
  - Halo particle update still needed at every time step.
  - Add skin radius.



ls1 mardyn

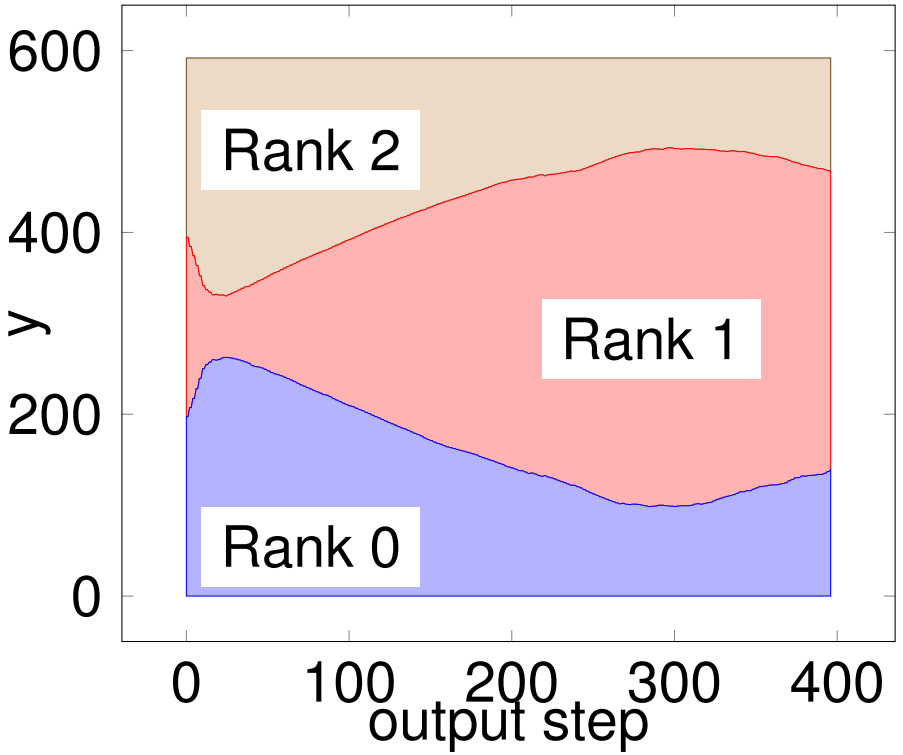
ls1 mardyn

- ls1 mardyn is an MD simulation package.
- Actively used in chemical engineering.
- Supports AutoPas as underlying particle container.



ls1 mardyn – MPI Adaptions

- Diffusive load balancing via library developed at JSC.
- Neighbor communication was adapted to AutoPas interface – allows efficient use of Neighbor lists.



Experimental Results

Conclusions

- AutoPas is a black box *N*-Body container.
- Dynamic tuning enables optimal performance for changing scenarios.
- Achievable for users without expert knowledge.
- Easy to integrate in existing codes.

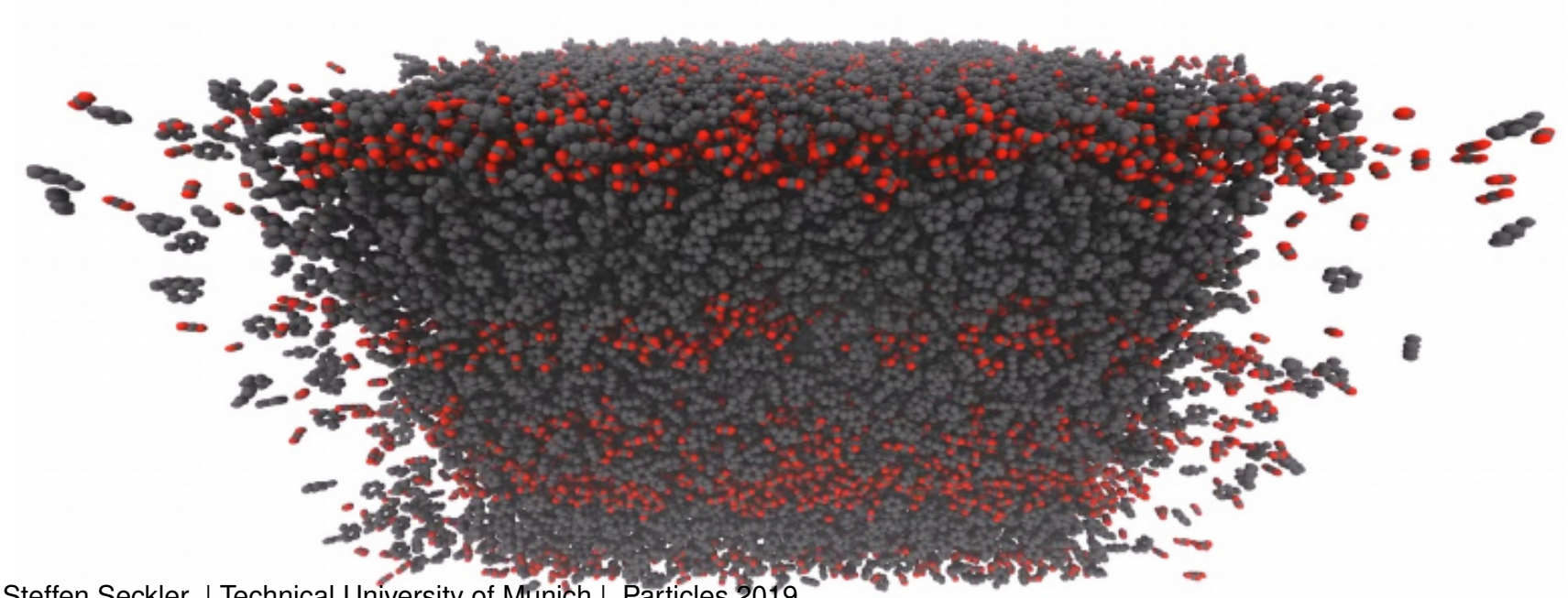
... and future work:

- Add more advanced auto-tuning strategies.
- More / optimized algorithms.
- Tuning for more parameters.
- Search space reduction.

Backup Slides

Molecular Dynamics

- Here: small rigid molecules
- Simulation of movement of molecules
- Computation of pairwise forces
- Newtons Laws of Motion
- N-Body problem $\Rightarrow O(N^2)$



Short Range Interactions: Lennard-Jones Potential

$$U(x_i, x_j) = 4\varepsilon \left(\left(\frac{\sigma}{||x_i - x_j||_2} \right)^{12} - \left(\frac{\sigma}{||x_i - x_j||_2} \right)^{6} \right) \tag{1}$$

- Characteristics of molecule type:
  - ε : Potential well
  - σ : Zero crossing
- Cutoff r_c

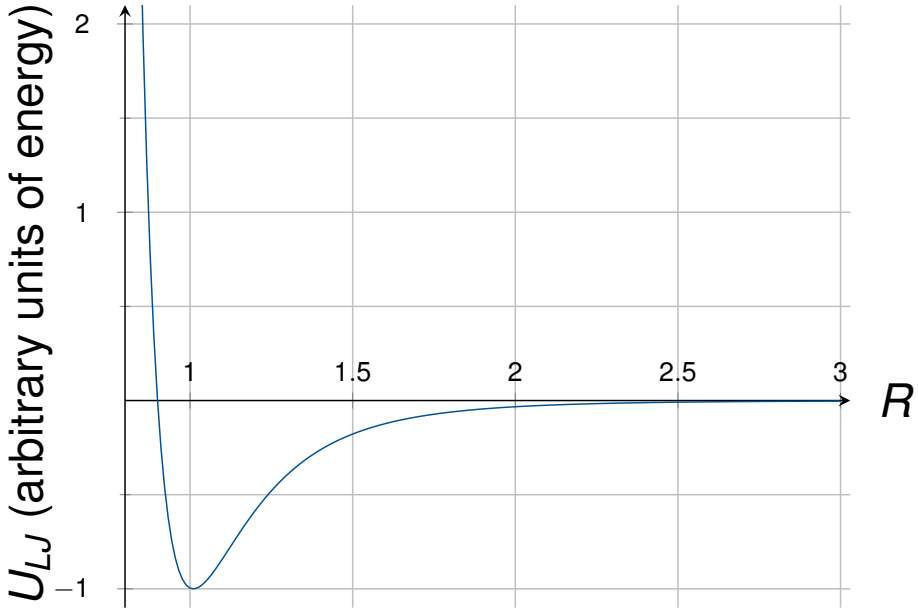
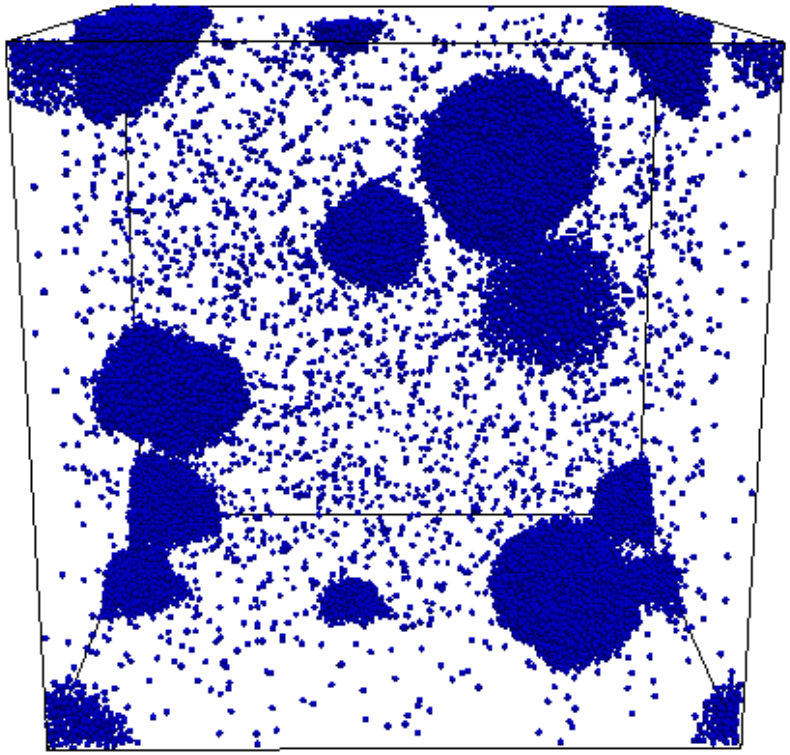


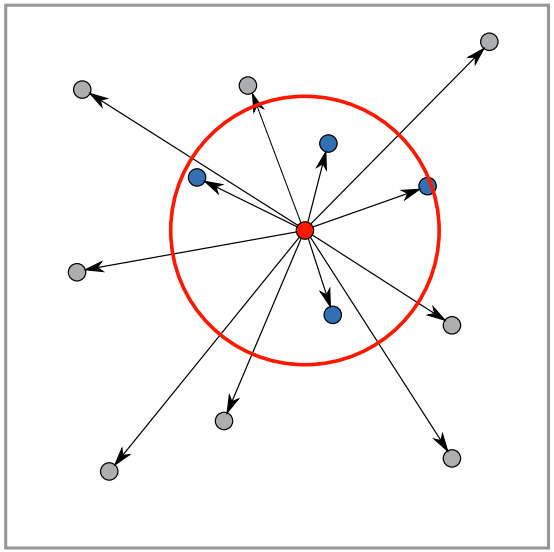
Figure: LJ-Potential for $\varepsilon = 1$ and $\sigma = 0.9$

Challenges

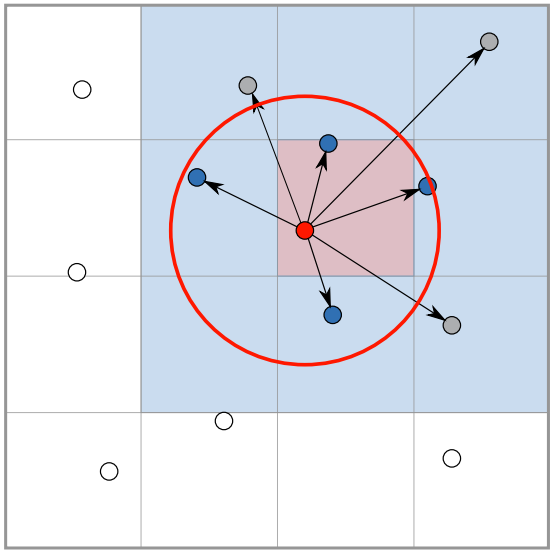
- Total number of particles
- Particle density
- (In-)Homogeneity
- Systems changing over time
- Many possible algorithms
- Overall goal:
  Minimize time to solution!



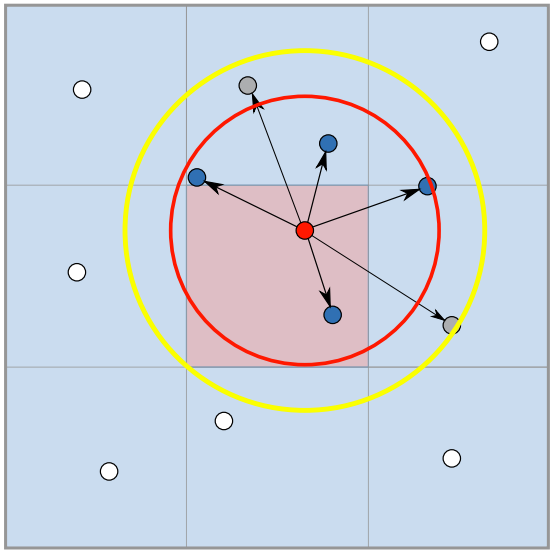
Container Options



Direct Sum



Linked Cells



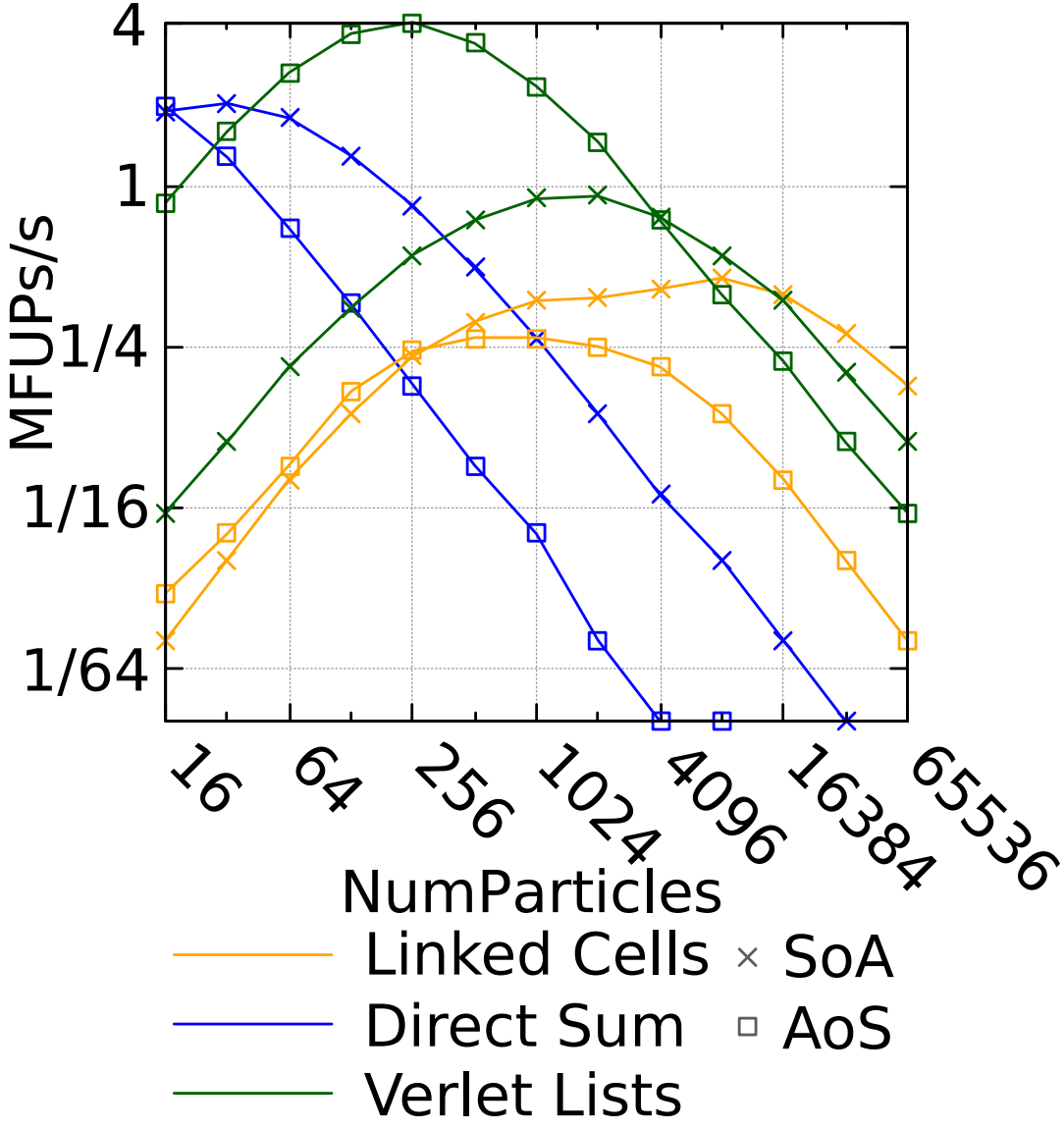
Verlet Lists

Memory Overhead

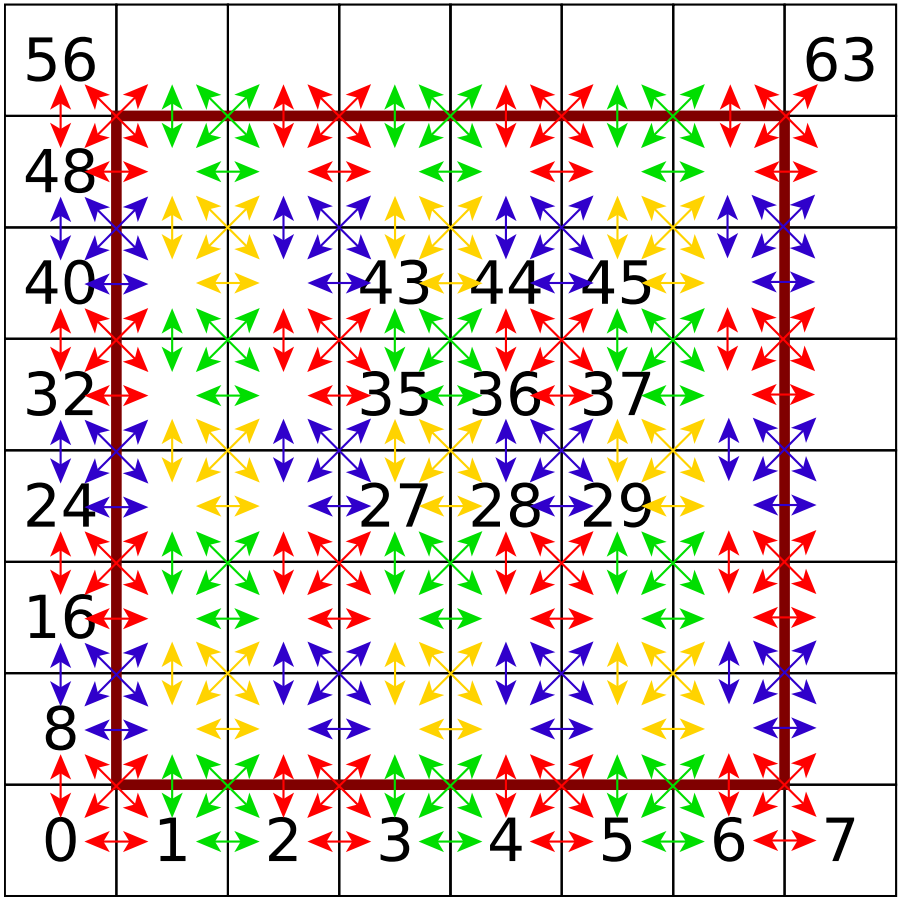
Computational Overhead

Container Comparison

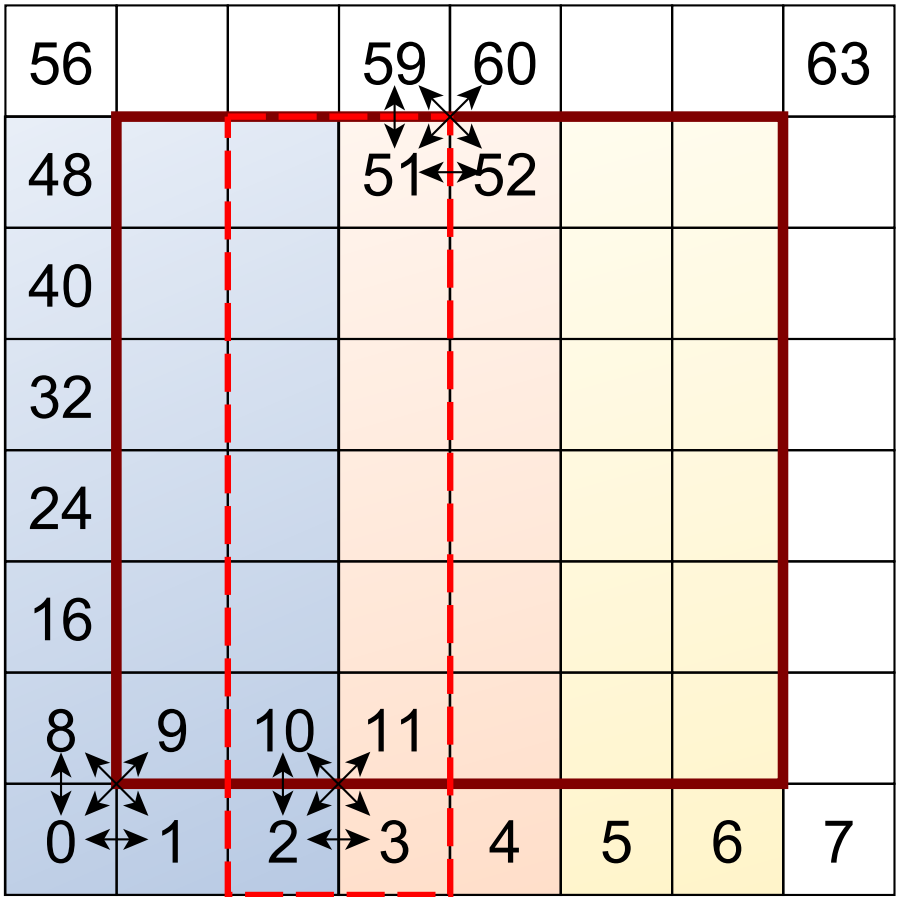
- Every container has advantages
- Linked Cell benefits most from SoA
  $\Rightarrow$best in dense scenarios



Linked Cells Parallelization Options



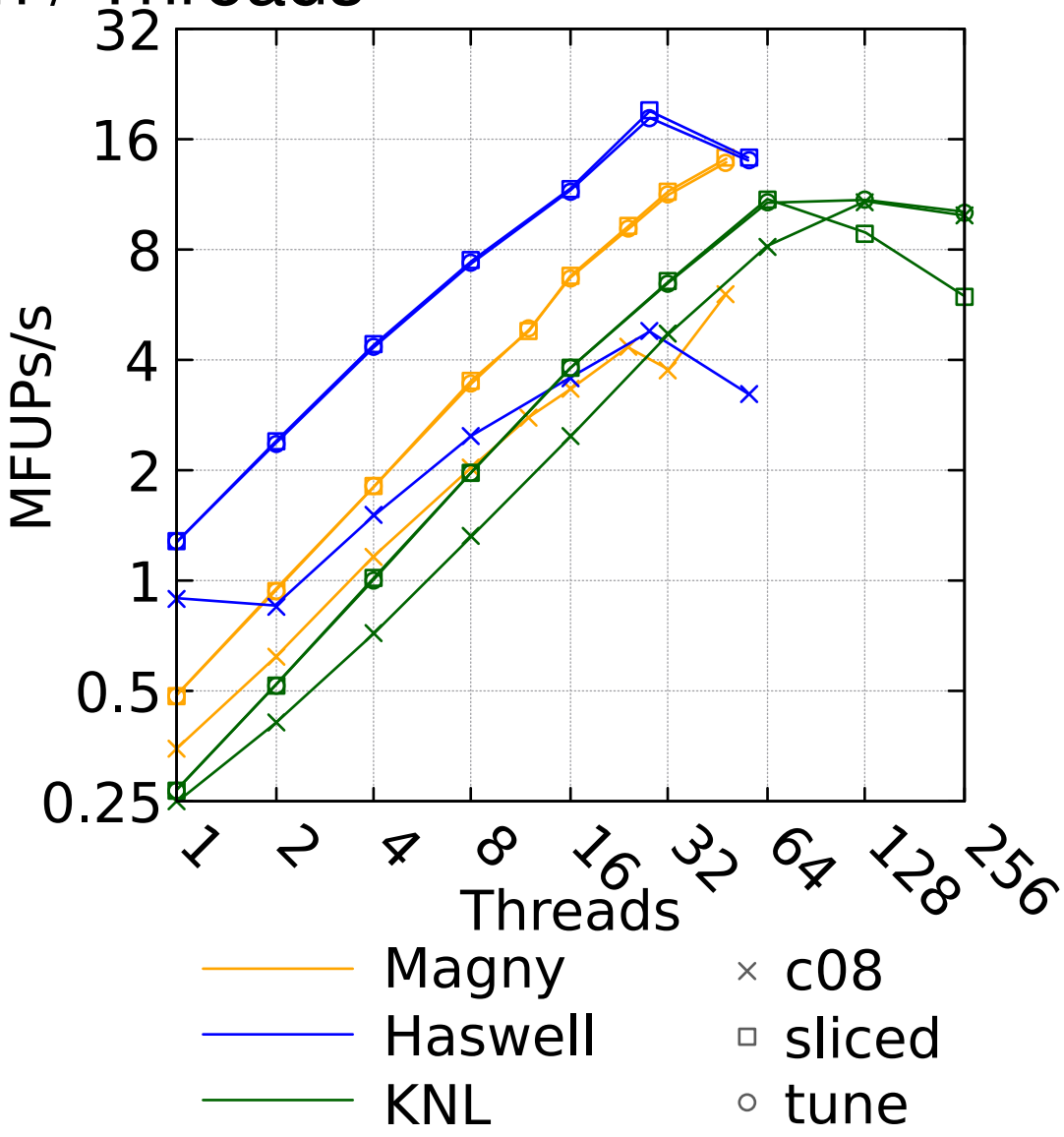
c08



sliced

Hardware Comparison / Threads

- Traversals:
  c08: 8-way domain coloring
  sliced: regular 1D domain partitioning

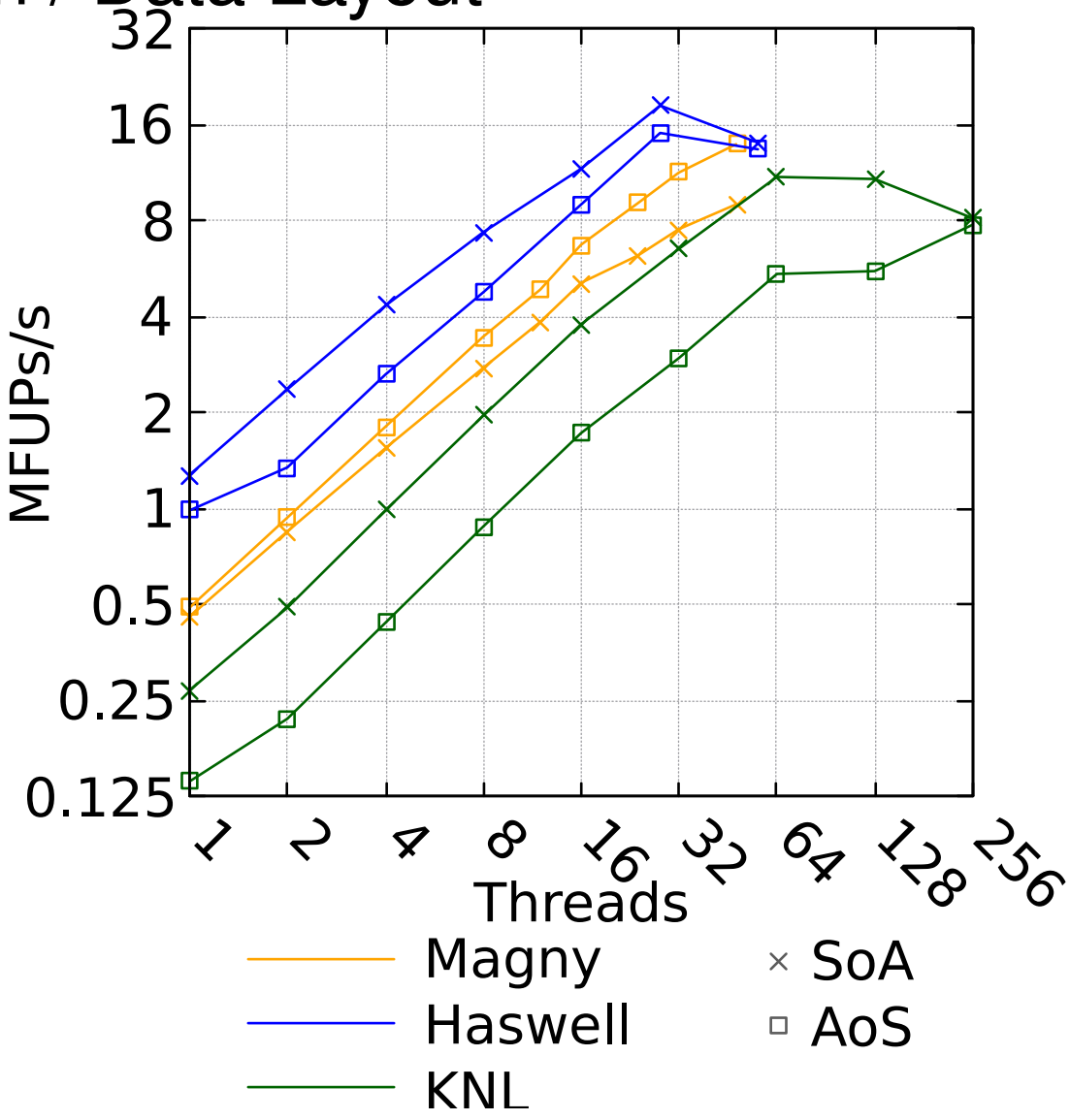


Hardware Comparison / Data Layout

- Vector Instructions:

Magny	SSE4	128
Haswell	AVX2	256
KNL	AVX512	512

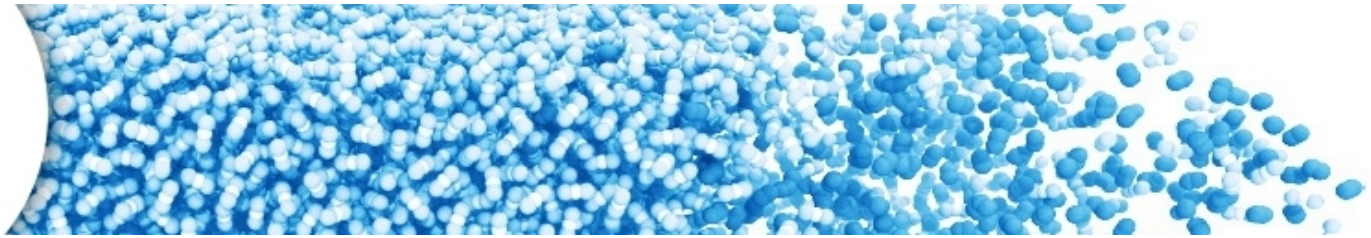
⇒ Optimal data layout dependent on hardware



AutoPas in ls1 mardyn

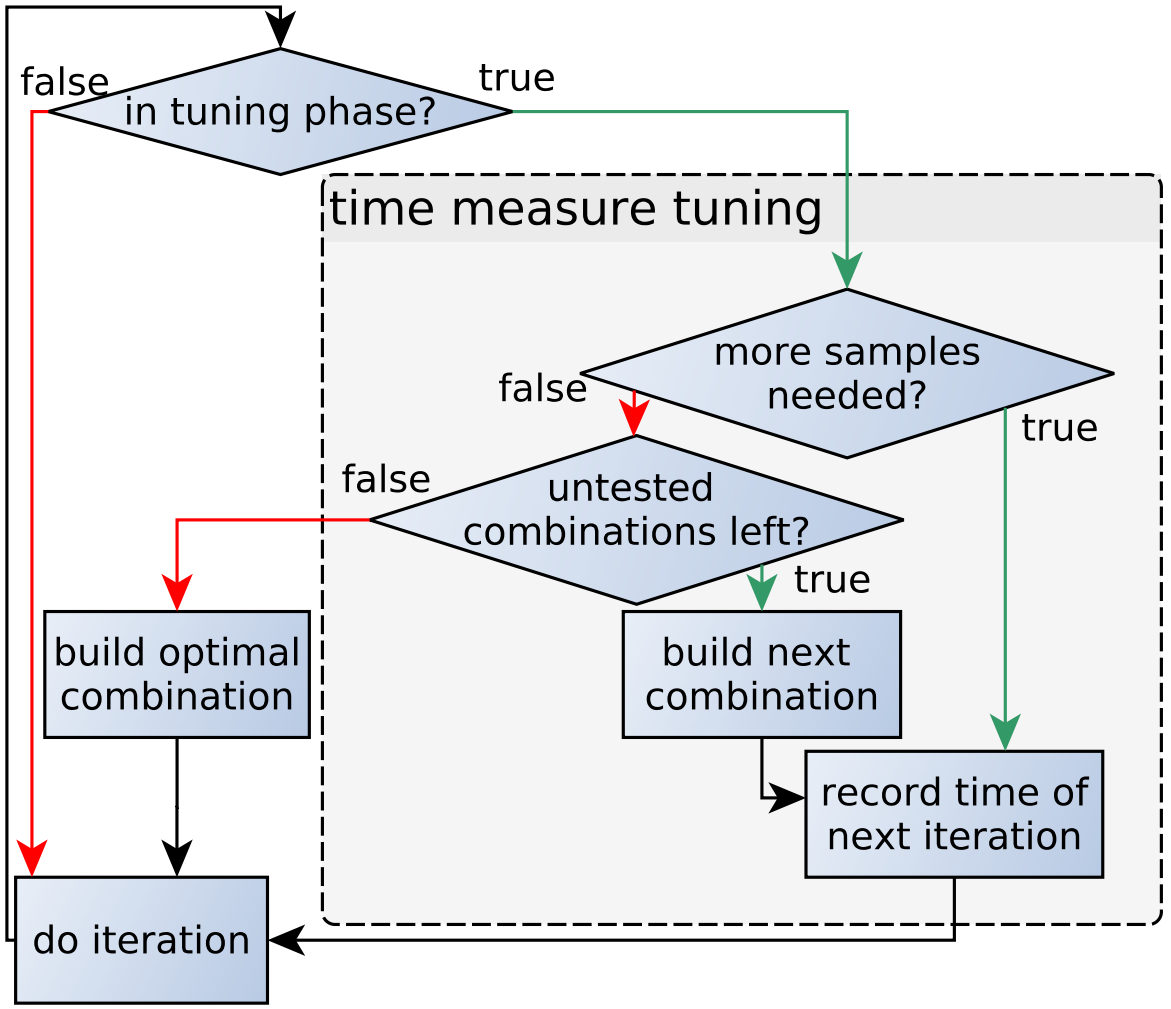
- Uses Lennard-Jones functor from AutoPas
- New particle class
  - Inherits from AutoPas and ls1 mardyn particle interface.
  - Acts as coupler
- New particle container class
  - Only wrapper around AutoPas main interface.

ls1 Mardyn



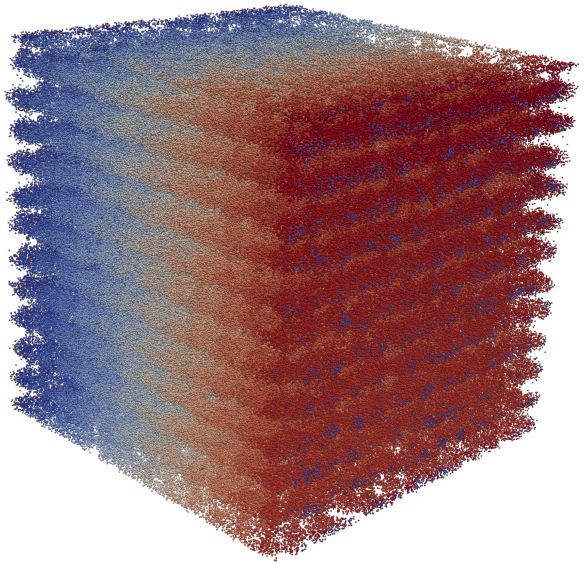
Auto-Tuning Process

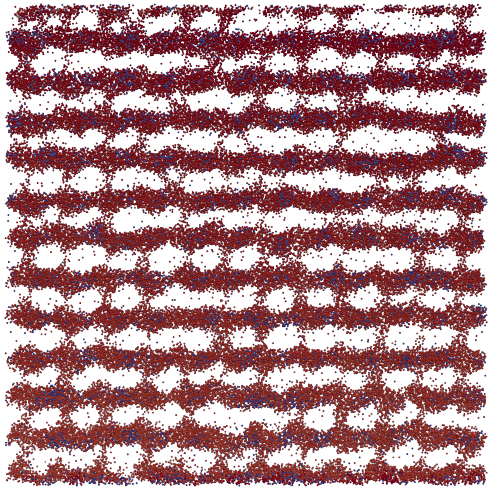
- Common interfaces for containers, traversals, etc
  $\Rightarrow$ Strategy pattern
- Repeated periodically
- User can restrict testing space



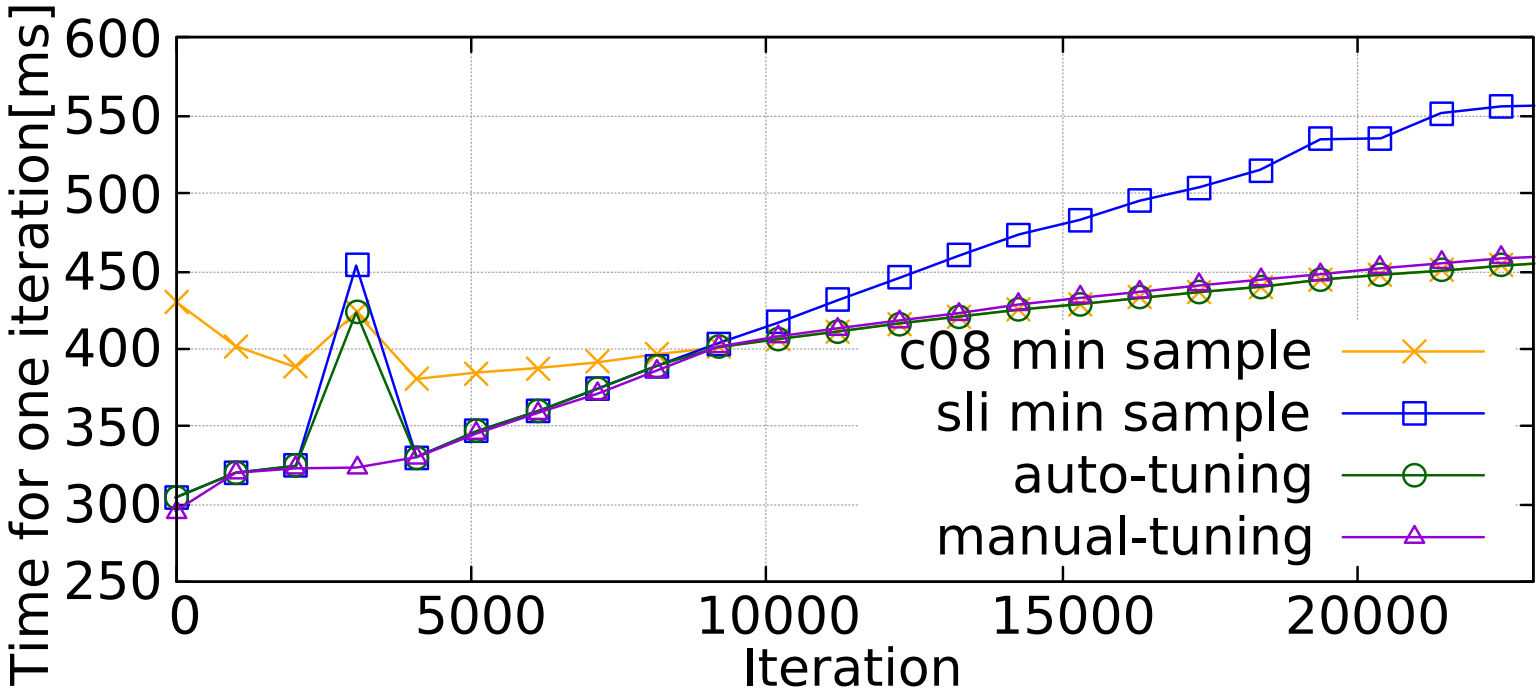
Scenario: Spinodal Decomposition

- 4 008 960 particles
- Block size: $240 \times 240 \times 240$
- Periodic boundary conditions
- Cutoff = 2.5
- Sub-critical temperature
- Rapid and drastic change in homogeneity
  $\Rightarrow$ Interesting target for tuning!



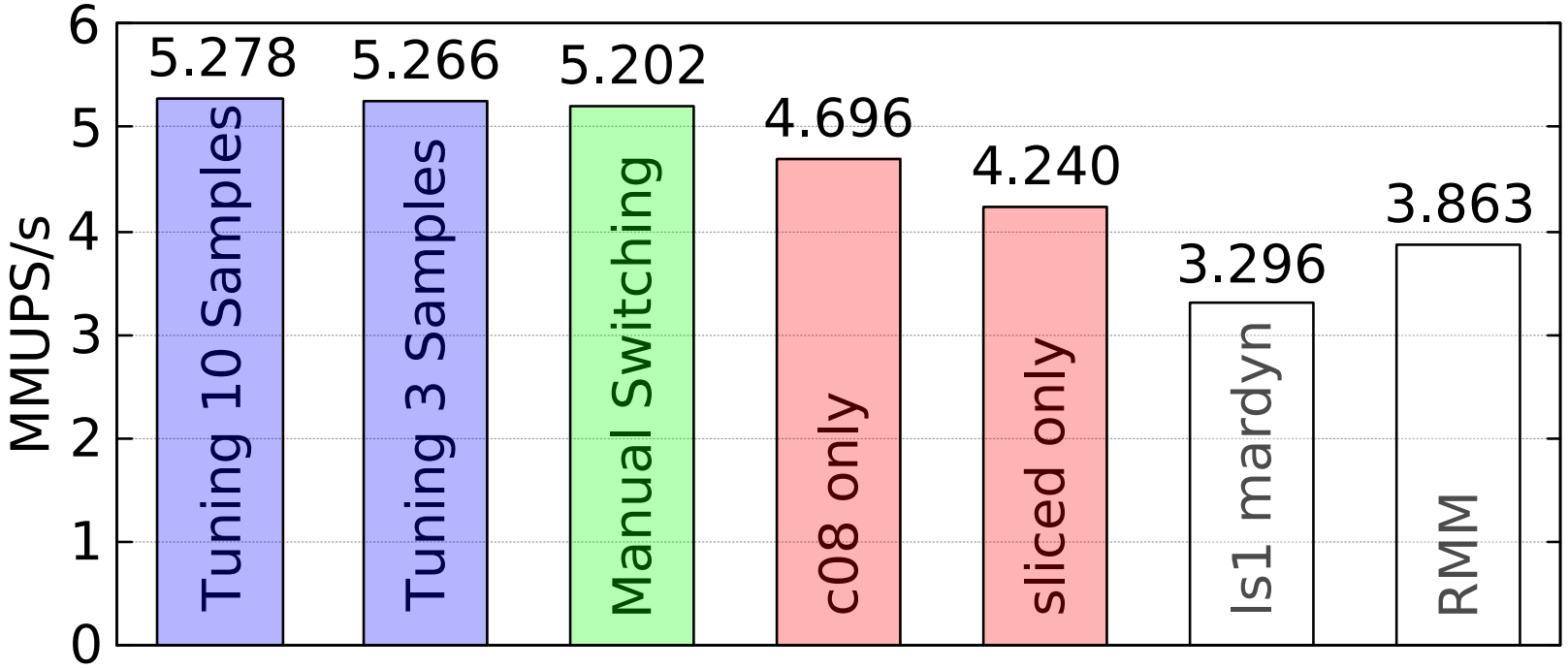


Tuning Behavior



- Tuning switches as expected
- Misclassification can happen

Tuning Overhead



- Tuning and manual switching equally fast.
  $\Rightarrow$ No overhead from tuning!
- Tuning faster than static configuration.
- Faster than original ls1 mardyn, even in Reduced Memory Mode.