AutoPas

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Simulation-Tuned Time and Energy Optimisation for Multi-Site and 3-body Molecular Dynamics Simulations with AutoPas

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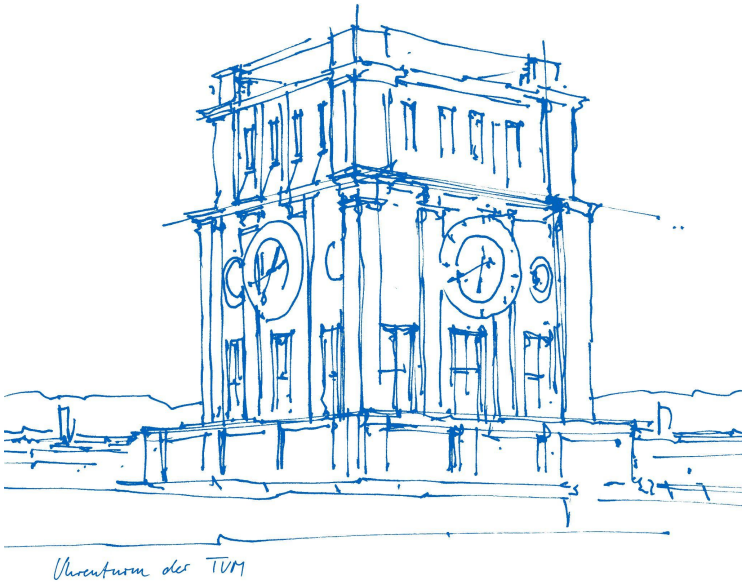

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What is the best algorithm for short-range Molecular Dynamics?

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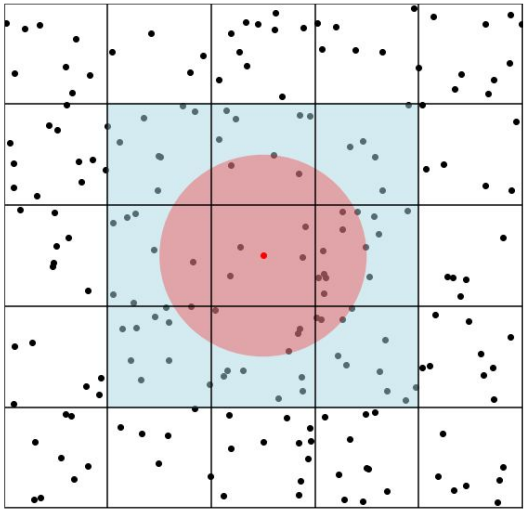
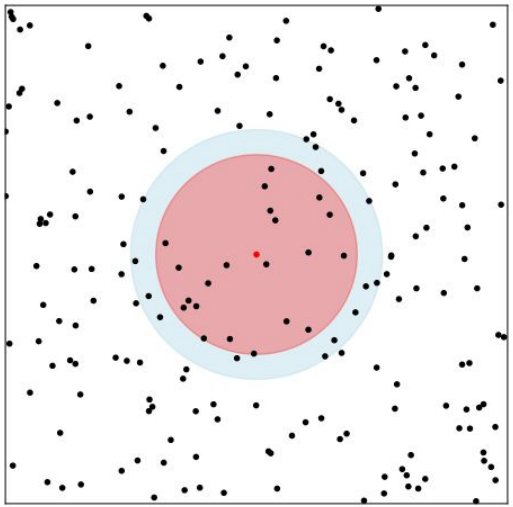
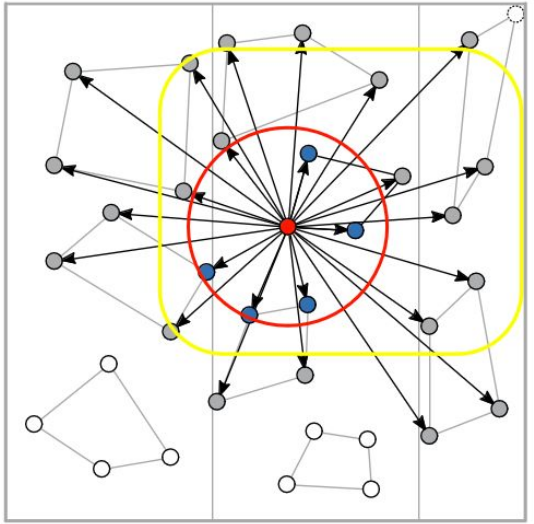
What is the best algorithm for short-range Molecular Dynamics?



Linked Cells

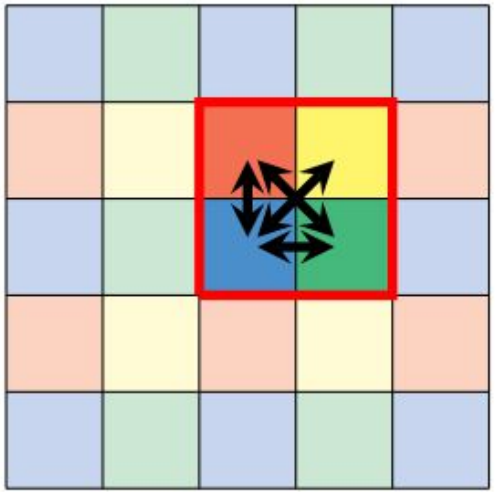


Verlet Lists

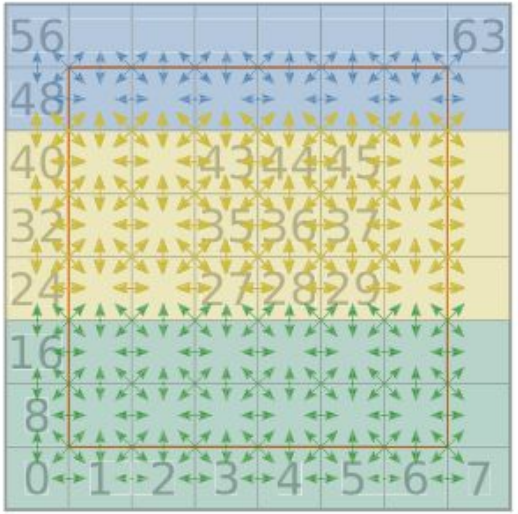


Verlet Cluster Lists

What is the best way to parallelism these algorithms?

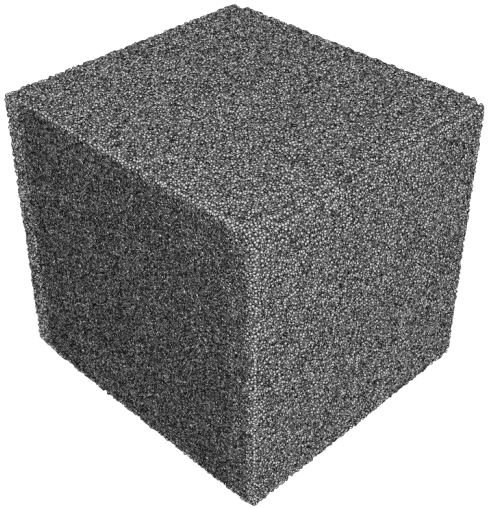


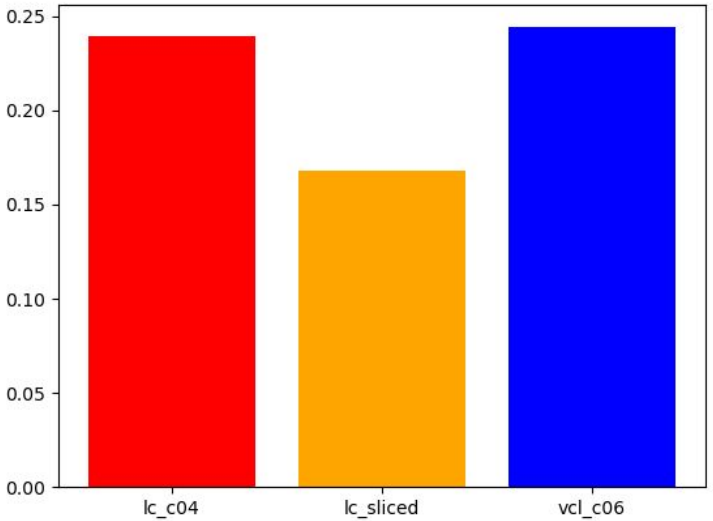
Colour-Traversals: Each colour can be traversed in parallel without race conditions



Slice-Traversals: Each slice is handled by a different thread with a lock to handle the “crossover” region

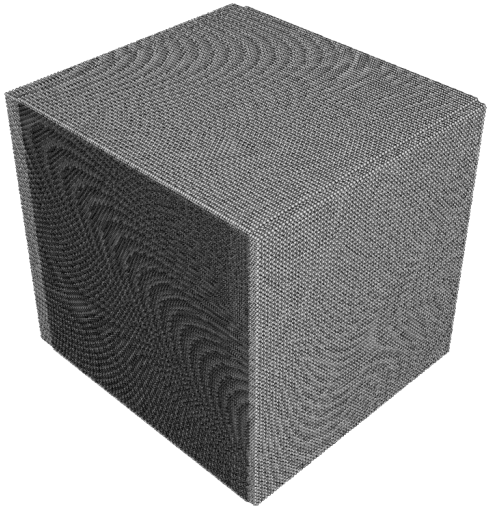
A Sparse Simulation

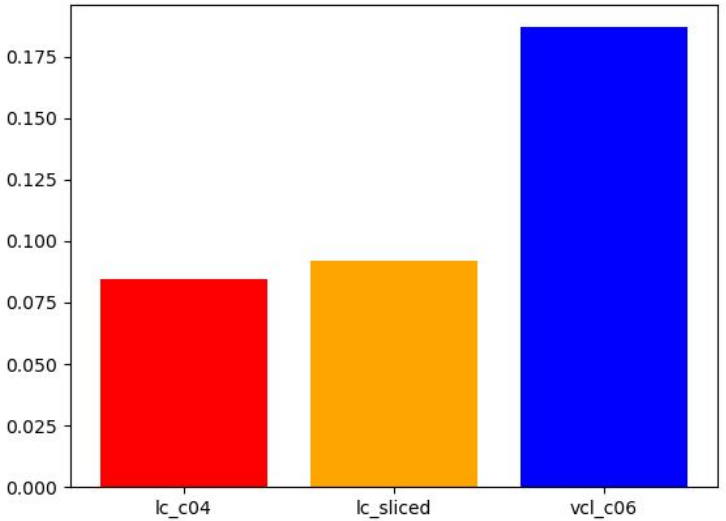




=> Linked Cells with a simple sliced parallelisation is fastest

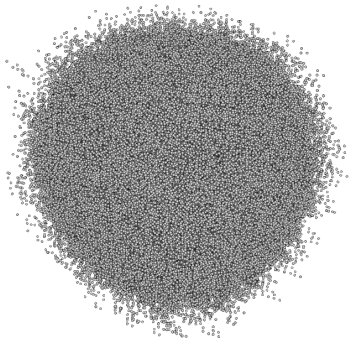
A Dense Simulation

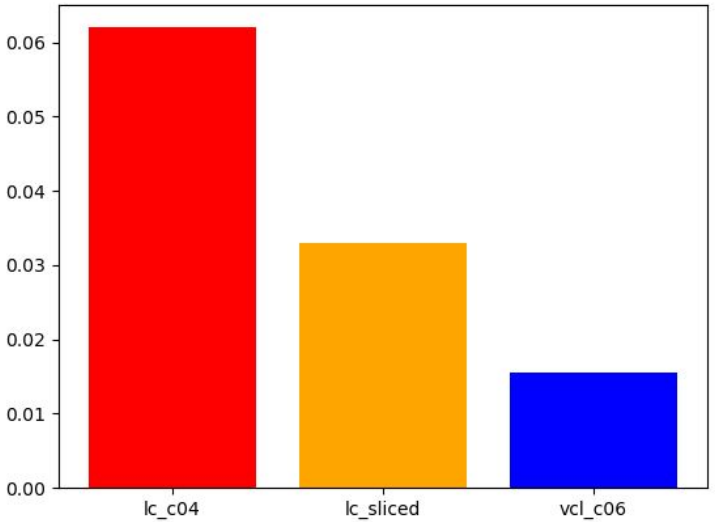




=> Linked Cells with a 4-coloured parallelisation is best

A Heterogeneous Simulation





=> Verlet Cluster Lists with a 6-colour parallelisation is best

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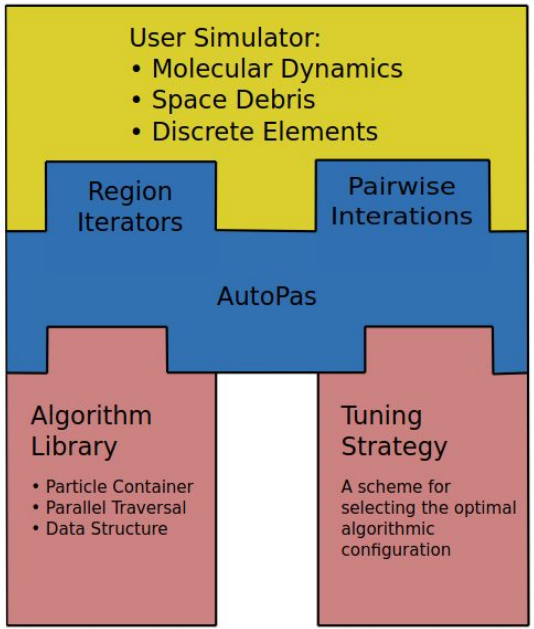
What if the simulation is changing?
Or different regions have different properties?

AutoPas: An algorithm-selection library for particle simulations

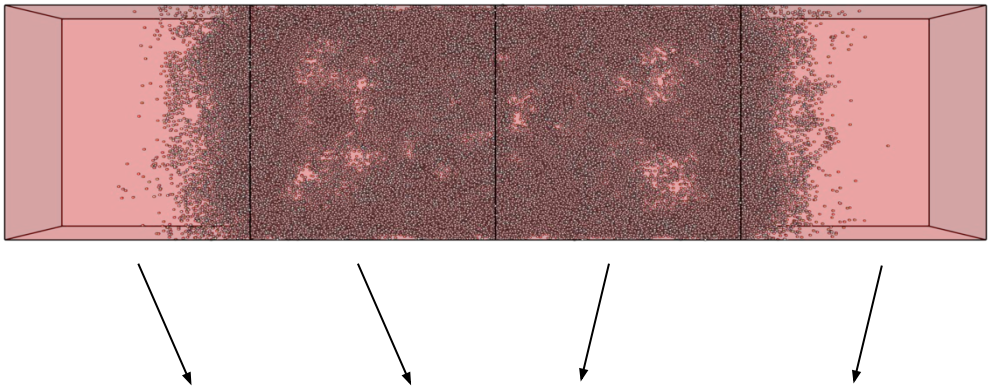
AutoPas is a black-box, rank-level particle simulation library for selecting the best algorithm for force-calculations:

- Contains an extensive library of algorithms and shared-memory parallelisations.
- Can change the algorithm as the simulation changes.
- “Black-box”: The developer of simulator does not need to consider what algorithm is optimal.
- Only support for CPU currently :(



AutoPas and MPI

AutoPas does not offer distributed memory parallelisation. A typical domain decomposition can be used with each rank having its own AutoPas container.



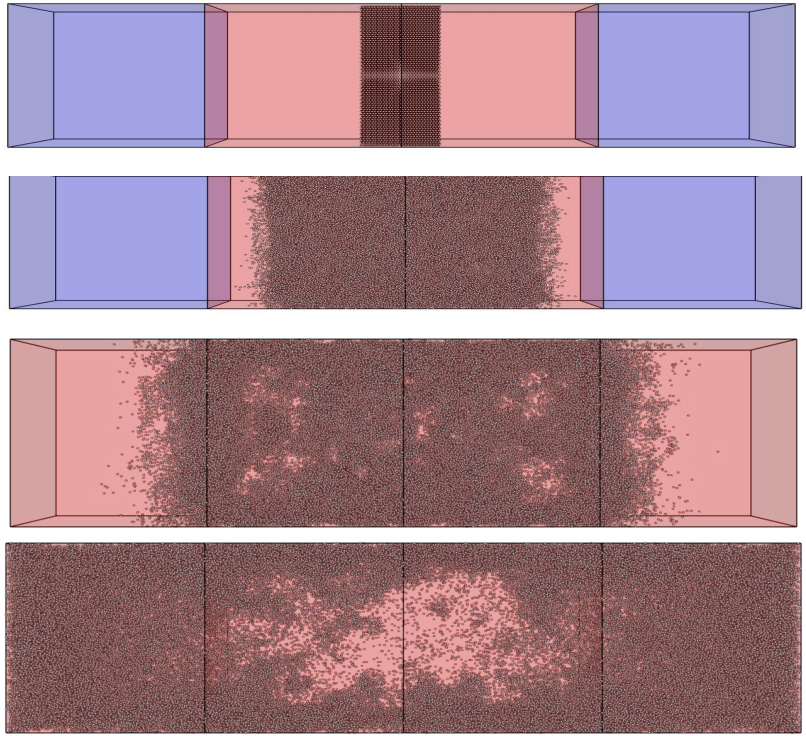
Each can make its own decision about which algorithm to choose

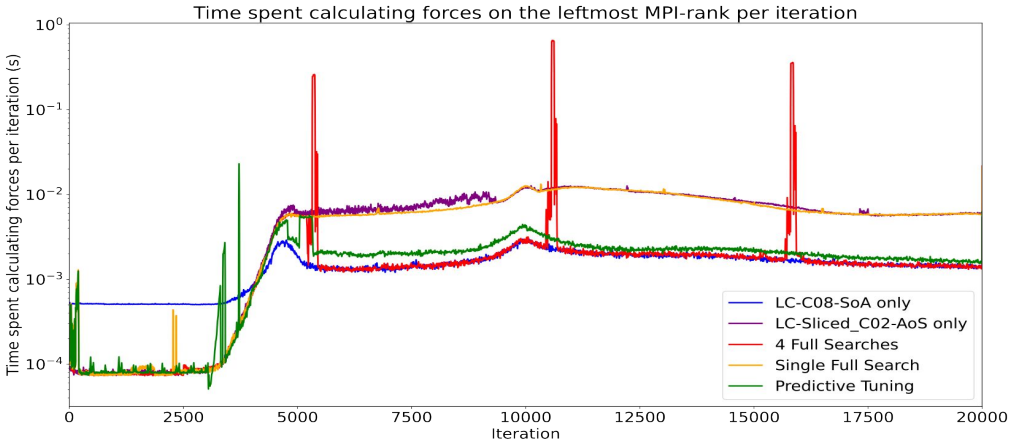
How do we select/tune the algorithms?

- We alternate between
  - Tuning phases which trial algorithmic/parameter combinations and select an optimal configuration.
  - Non-tuning phases which use that optimum.
- We can tune for optimal time or optimal energy consumption*.
- Tuning strategies reduce the number of algorithmic configurations that are trailed. These are still works-in-progress.

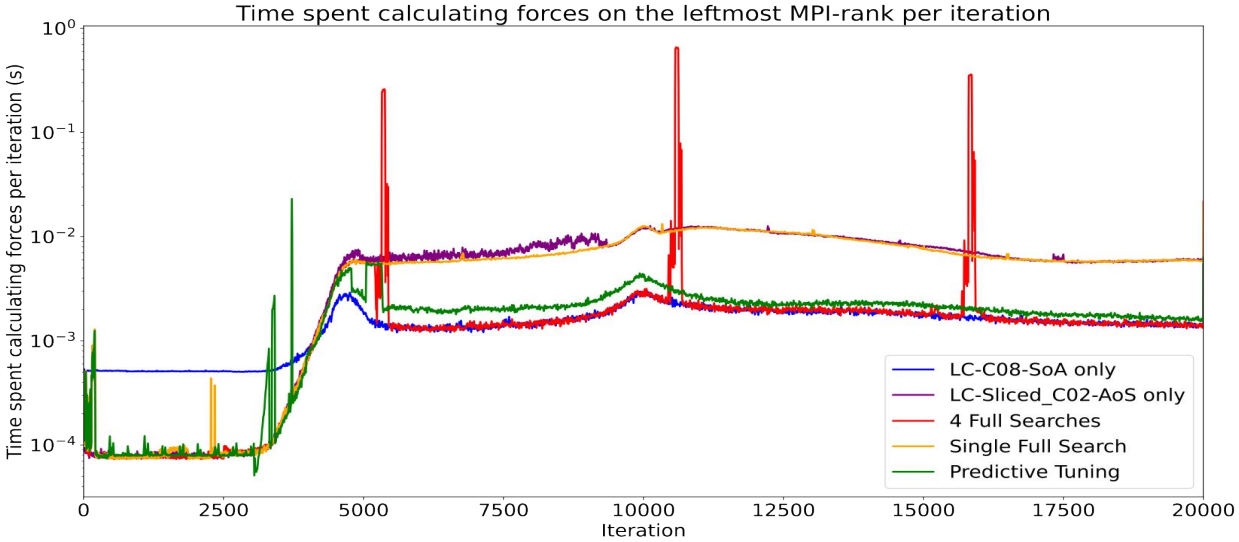
*only on Intel processors

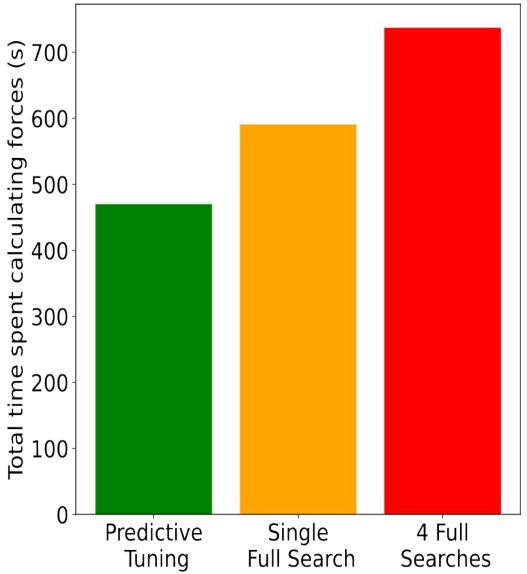
Example: Exploding Liquid





Example: Exploding Liquid





Future Work

- Better tuning strategies!
  - Decision Trees
  - Fuzzy Logic Approaches
- Energy measurements (or surrogates) on non-Intel architectures.
- GPU support
  - Through either Kokkos or SYCL

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Applying AutoPas to specialised Molecular Dynamics topics

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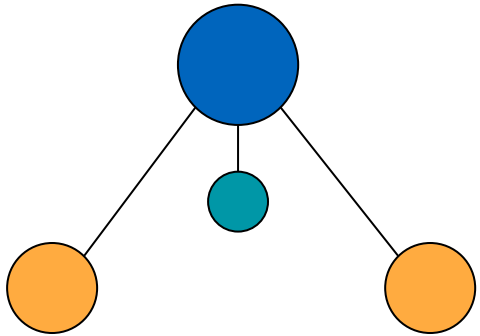
Multi-Site Molecular Dynamics

- Small rigid body molecules consisting of Lennard-Jones and Electrostatic Sites.
- Forces calculated between inter-molecular pairs of sites leading to total forces + torques.
- Used in thermodynamics-focused MD simulators (e.g. ls1-MarDyn)



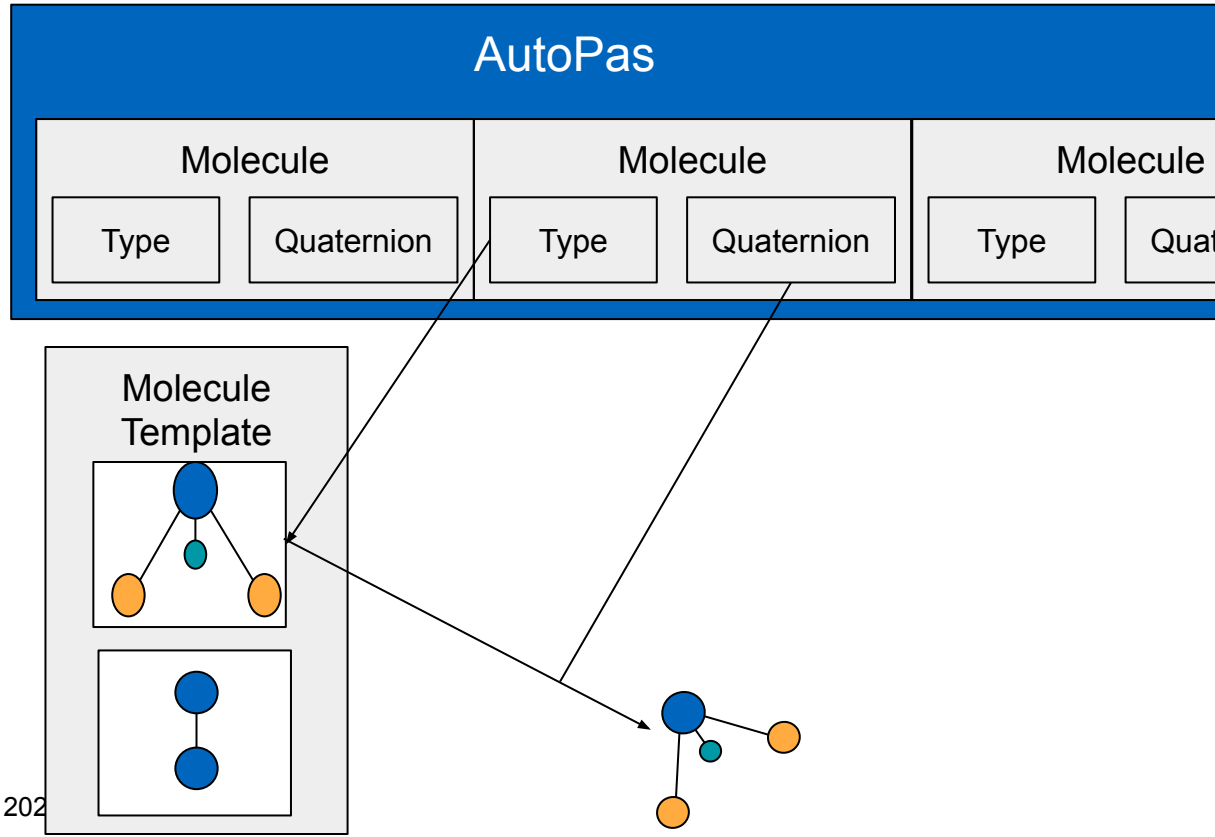
The goal:

- Effective application of all our algorithms to this type of simulation.
- Dynamically select different algorithms for Lennard-Jones and Electrostatic force calculations.

Multi-Site Molecular Dynamics

Template Approach:

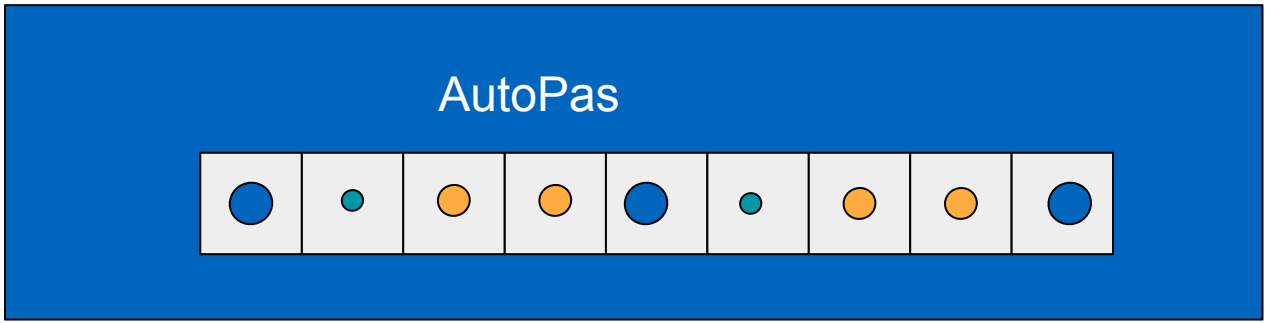
- AutoPas stores molecule types and quaternions.
- During force calculation: Molecule types are used to lookup molecule templates which are rotated with a quaternion.
- Pro: Low Memory footprint per molecule
- Con: Frequent (Re-)Computation of exact site positions required.



Multi-Site Molecular Dynamics

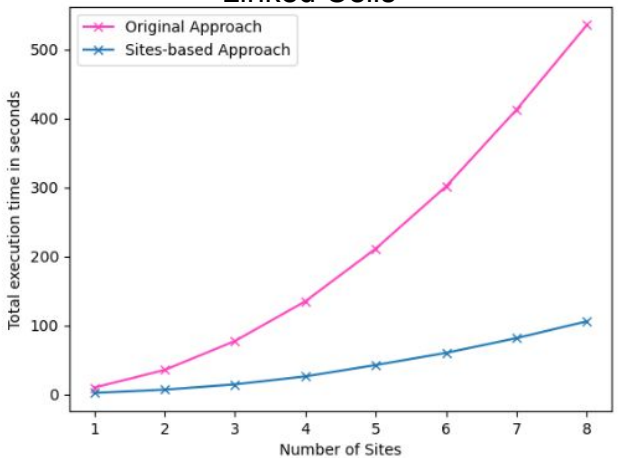
Exact-Site Position Approach Approach:

- AutoPas stores sites directly and for each site, we keep track of which molecule it belongs to.
- Pro: Nice for pipelining
- Cons: Management overhead and higher memory footprint

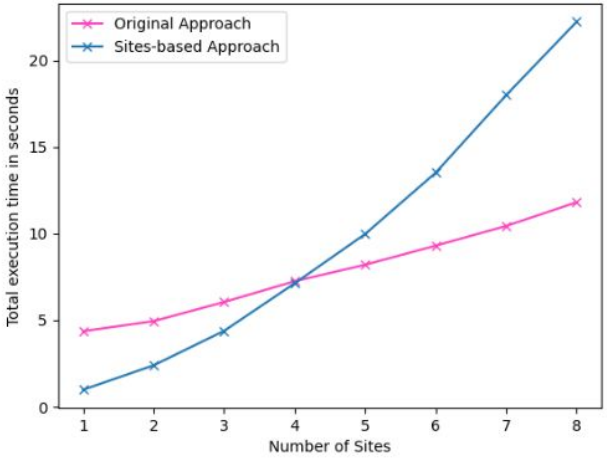


Multi-Site Molecular Dynamics: Preliminary Results

Linked Cells



Verlet Lists



Experimental results by Johannes Riemenschneider.

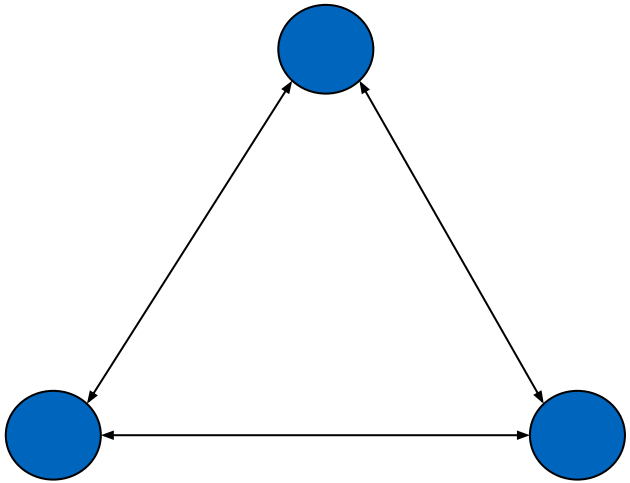
21x21x21 domain with a density of 0.87.

Simulation run on CoolMUC-2.

- Directly storing sites performs well (in some cases)
- But not suitable with MPI and some algorithmic/scenario combinations
- Perhaps a hybrid approach??

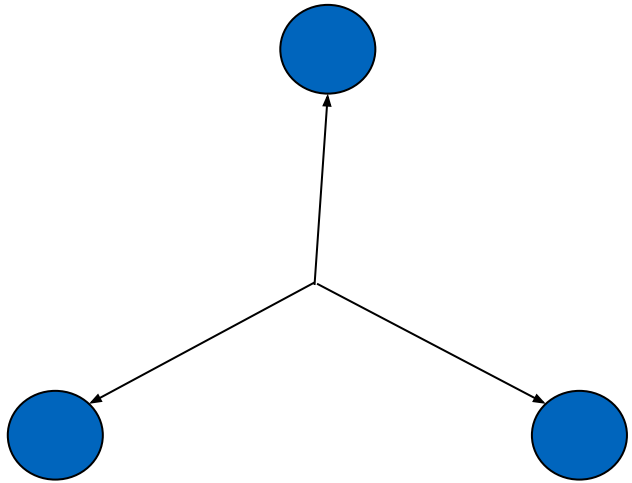
3-body Molecular Dynamics

- Previous only considered forces based on pairs of particles.



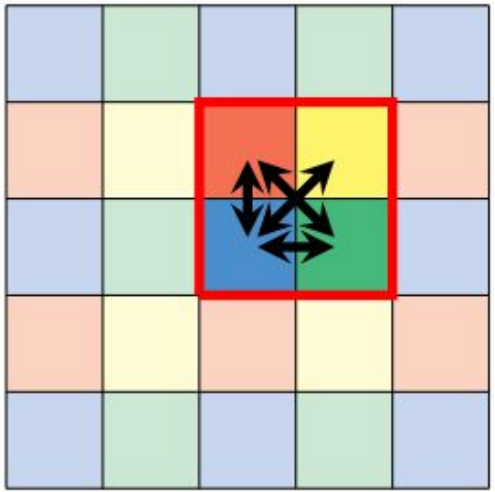
3-body Molecular Dynamics

- Previous only considered forces based on pairs of particles.
- For greater accuracy, “corrector” forces based on triplets of particles can be used.
- E.g. The Axilrod-Teller-Muto Potential



3-body Molecular Dynamics

- Colour-traversals of Linked Cells for 3-body interactions have been developed.
- A Verlet-based approach is in the process of being developed.
- AutoPas' tuning mechanism has been extended to allow for separate algorithms to be chosen for 2-body and 3-body interactions.



Example: 8-colour Linked Cells Traversal - Each colour can be traversed in parallel without race conditions

Acknowledgements

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- Manish Mishra
- Many students of TUM

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- HSUper
- CoolMUC-2

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Federal Ministry of Education and Research

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Summary

- Motivated and introduced the black-box simulation library AutoPas.
- Discussed adaptations of AutoPas for specialised MD simulations.
- Key future directions include GPU support and better tuning.

GitHub:

References:

Contact: samuel.newcome@tum.de