
Seminar Final Presentation

Algorithm Selection and Auto-Tuning in AutoPas

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Software Challenges in Molecular Dynamics

- Enormous numbers of particles
 - naively: $\mathcal{O}(N^2)$ interactions
- Solution: highly optimized algorithms
 - Make full use of hardware
 - Smart data structures
- Every millisecond counts

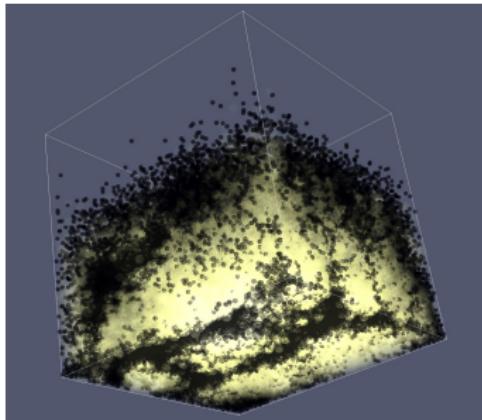
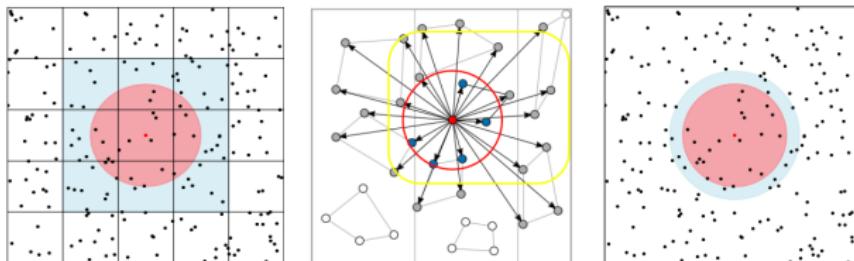


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Example: Particle Container

- How to identify interacting particles?
- Short-range forces allow for cutoff radius $\rightarrow \mathcal{O}(N)$ interactions
- Different implementations possible



Linked Cells

Verlet Cluster Lists

Verlet Lists

Simpler Memory Access

Lower Memory Overhead

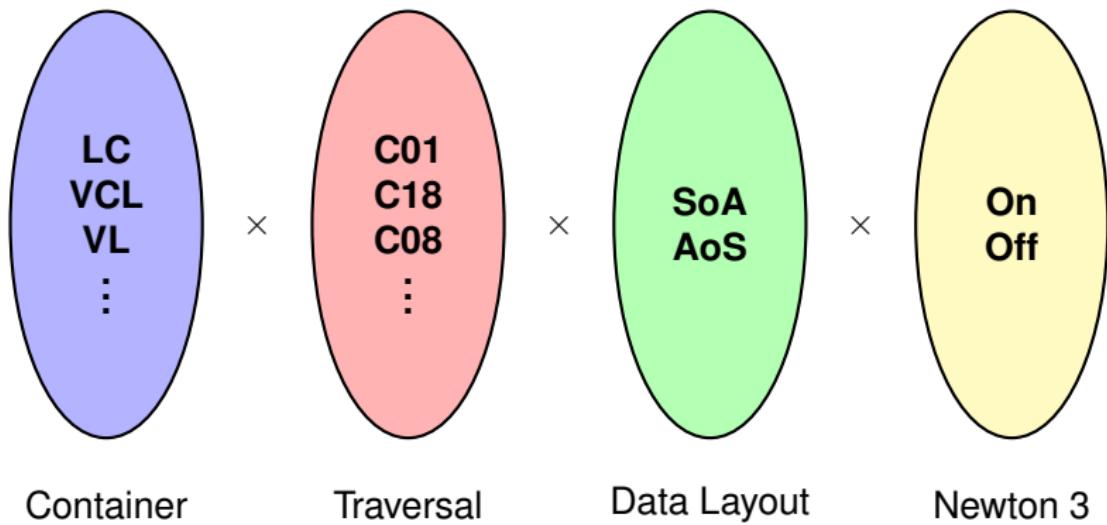
Fewer redundant calculations

Many more difficult choices

- Shared memory traversals
- Data layouts
- Newton 3 optimization
- ...
- Best choice depends on:
 - Hardware
 - Scenario

Which Combination to Choose?

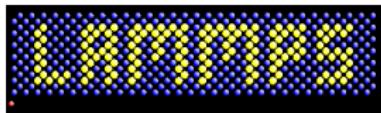
- Remember: No silver bullet!



Traditional MD Engines



- Based on a single combination
- Performance through:
 - Very optimized code
 - Vectorization
 - Manual tuning to target hardware
- Drawbacks:
 - Suboptimal for some scenarios
 - Manual tuning effort



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AutoPas

What is AutoPas?

- Library for arbitrary N-body simulations
- Implements all algorithms
 - Modular
 - All* configurations possible
- Idea: AutoTuning
 - Finds optimal configuration
 - Runtime switching
 - Thus optimal performance
- Arbitrary user code

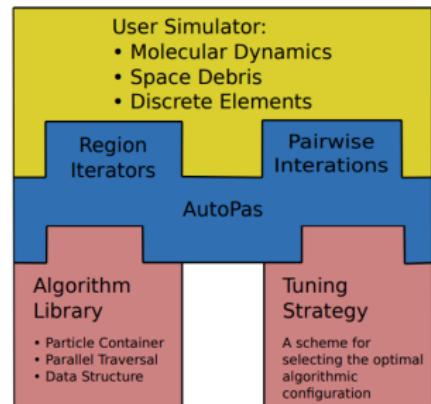


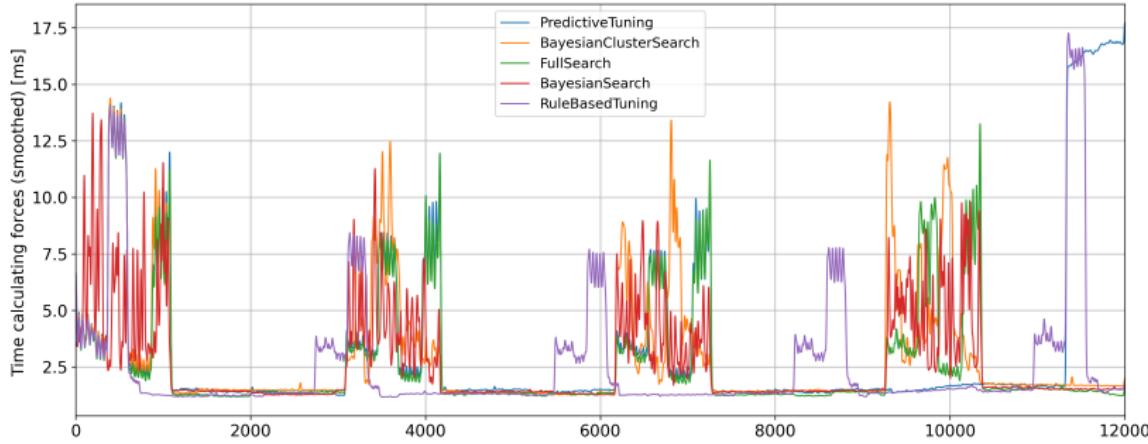
Figure: [Newcome et al., 2023]

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Auto-Tuning in AutoPas

- Tuning-Phase: Evaluate promising configurations
- Simulation-Phase: Use best configuration
- Capable of reducing simulation time!



Problems of Auto-Tuning

- Overhead from evaluating suboptimal configurations
 - Orders of magnitude slower!
- Unnecessary periodic re-tuning

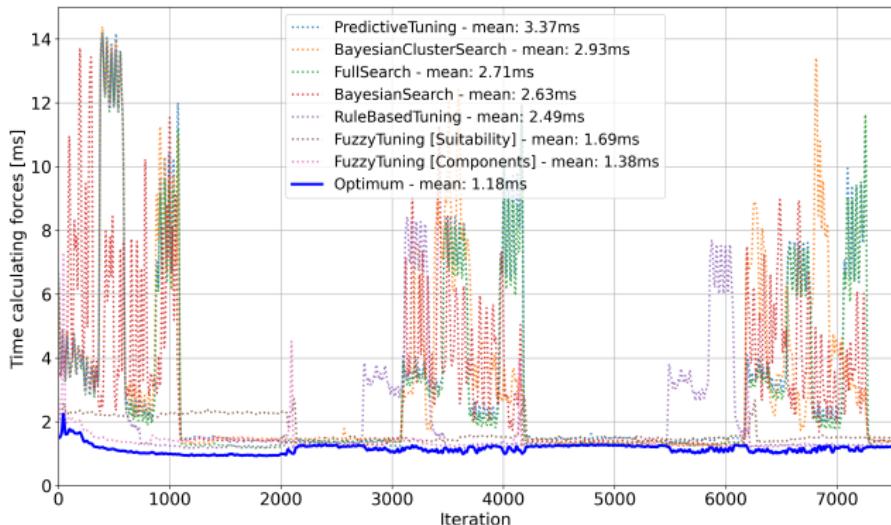
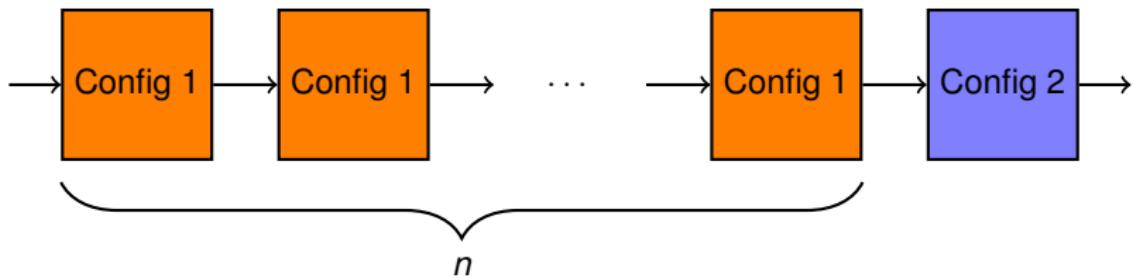


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Early Stopping Optimization

- Idea: Stop long-running evaluations early
- Configurations get sampled multiple times
- Naive approach:
 - Last sample performed poorly?
 - Stop further evaluations

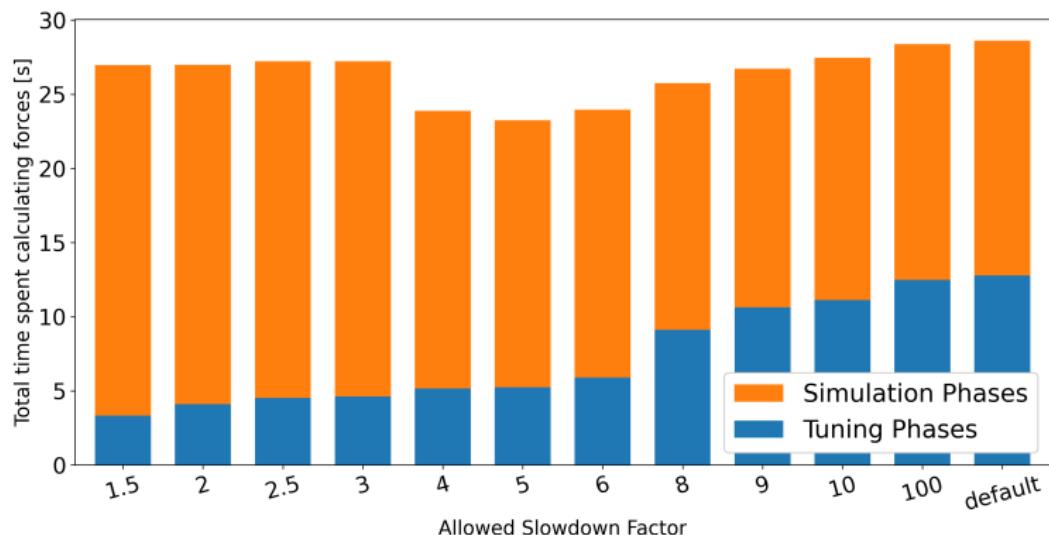


Naive Early Stopping

- Changes to AutoPas are minimal
 - Keep track of best performance seen so far
 - $\text{slowdownFactor} = \frac{t_{\text{sample}}}{t_{\text{best}}}$
 - Call `retune()` if `slowdownFactor` exceeds threshold
- Hyperparameter: *allowedSlowdownFactor*
- Which *allowedSlowdownFactor* should be used?
 - *allowedSlowdownFactor* → 1: Many aborts
 - *allowedSlowdownFactor* → ∞: No early stopping
- Empirical evaluation needed

Benchmark: Exploding Liquid + Predictive Tuning

- Optimal at $allowedSlowdownFactor = 5$
- From 28.6s to 23.2s
 - 18.9% reduction



Discussion of Naive Early Stopping

- Works well with good tuning strategies
 - t_{best} converges faster
- *allowedSlowdownFactor* probably not universal
 - More benchmarks needed!
- Investigate less naive approaches
 - Improve stopping criterion
 - Abort during evaluation

Thank you for your attention!

Questions?

References I

-  Newcome, S. J., Gratl, F. A., Muehlhaeusser, M., Neumann, P., and Bungartz, H.-J. (2024). Autopas: Dynamic algorithm selection in molecular dynamics for optimal time and energy.
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-  Newcome, S. J., Gratl, F. A., Neumann, P., and Bungartz, H.-J. (2023). Towards the smarter tuning of molecular dynamics simulations.
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