Chair of Scientific Computing
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Bachelor Thesis Final Presentation

Exploring Fuzzy Tuning Technique for Molecular Dynamics Simulations in AutoPas

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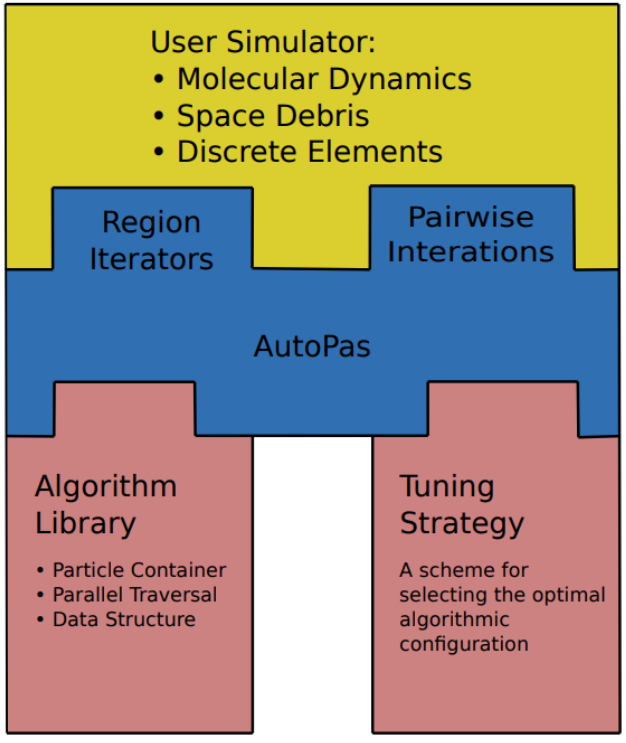
AutoPas

What is AutoPas?

- Library for optimal node-level performance in N-body simulations
- Many different implementations for the N-body problem
- AutoTuning: Automatically switch between implementations
  - **Container:** How to find neighboring particles?
  - **Traversal:** How to handle multi-threading?
  - **Data Layout:** How to store particles in memory?
  - **Newton 3:** Can we exploit Newton's 3rd law?
  - ...
- Example applications:
  - `md_flexible` (Molecular Dynamics)
  - `sph` (Smoothed Particle Hydrodynamics)

Structure of AutoPas

- Three main components:
  - User Application
  - Algorithm Library
  - Tuning Strategies
- Algorithm Library:
  - Huge Search Space[1]
- Tuning Strategies:
  - Full Search
  - Random Search
  - Predictive Tuning
  - Bayesian Search
  - Rule Based Tuning

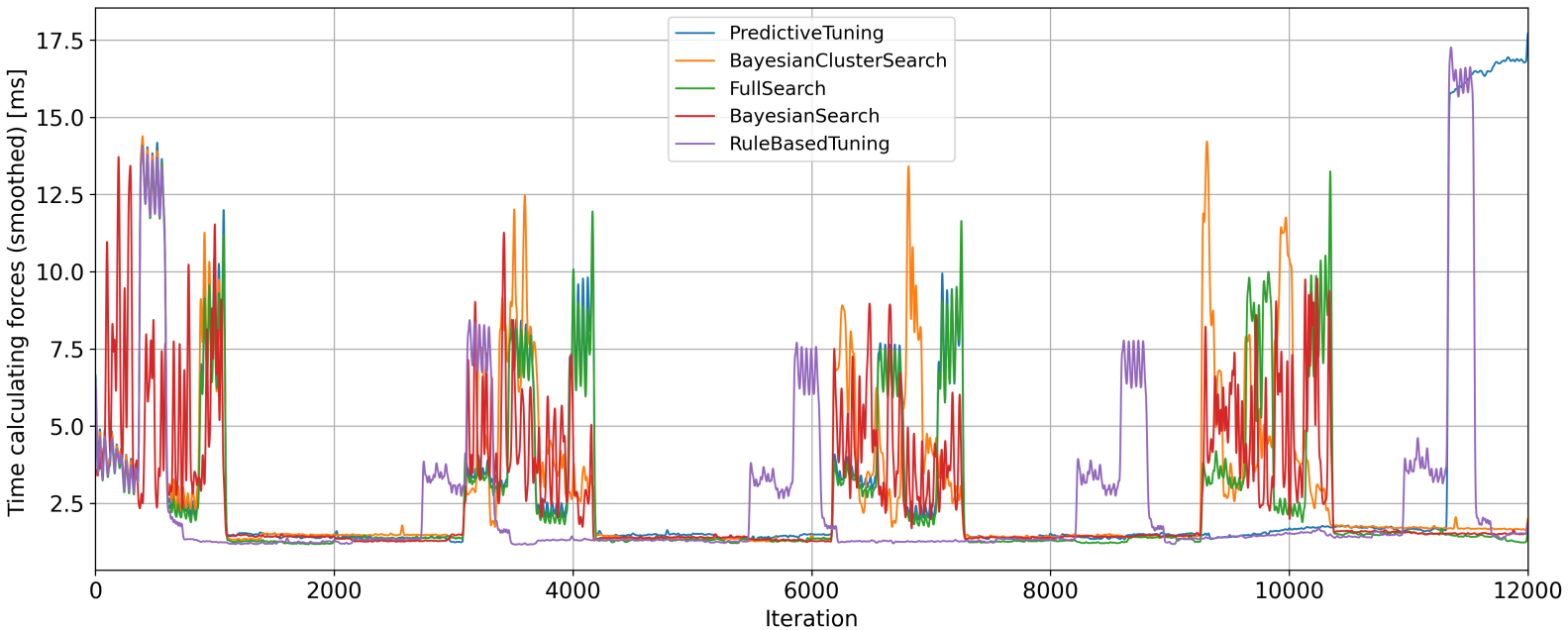


Source: [Newcome et al., 2023]

[1] Container × Traversal × Data Layout × Newton 3 × Load Estimator × Cell Size Factor

Auto-Tuning

- Tuning Phase: Find the best configuration
  - Tuning Strategies select configurations to evaluate
  - Fastest configuration wins
  - Expensive, Time consuming
- Simulation Phase: Use the best configuration



Fuzzy Tuning Strategy

- Benefits of Fuzzy Logic
- Recap of Fuzzy Logic concepts
- Application of Fuzzy Logic in AutoPas

Implementation

- Fuzzy Logic Framework
- Specification via Rule File
- OutputMapper

Proof of Concept

- Data-Driven Rule Extraction
- Fuzzy Systems for md flexible

Comparison and Evaluation

- Exploding Liquid Benchmark
- Spinodal Decomposition MPI
- Further Analysis

Future Work

- Dynamic Rule Generation
- Improving Tuning Strategies
- Simplification of the Fuzzy System

Conclusion

- Summary of Findings
- Impact
- Final Thoughts

References I


Newcome, S. J., Gratl, F. A., Neumann, P., and Bungartz, H.-J. (2023).
Towards the smarter tuning of molecular dynamics simulations.
Amsterdam, The Netherlands.