

Bachelor Thesis Final Presentation

Exploring Fuzzy Tuning Technique for Molecular Dynamics Simulations in AutoPas

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Introduction

- AutoPas
 - What is AutoPas?
 - Significance in particle simulation
 - Benefits of Tunable Parameters
 - Overview of Tunable Parameters
- Tuning strategies in AutoPas
 - Pruning the search space
 - Dealing with potentially bad configurations
 - Importance of efficient tuning strategies

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