Chair of Scientific Computing in Computer Science
Univ.-Prof. Dr. Hans-Joachim Bungartz

Technische Universität München

Bachelor Thesis Final Presentation

Exploring Fuzzy Tuning Technique for Molecular Dynamics Simulations in AutoPas

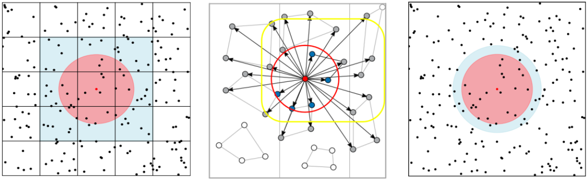
Manuel Lerchner
manuel.lerchner@tum.de

Advisors:
Manish Kumar Mishra, M.Sc.
Samuel James Newcome, M.Sc.

Table of Contents

What is AutoPas?

- Library for arbitrary N-body simulations
- Optimal performance by switching implementations
  - **Container:** Finding neighboring particles
  - **Traversal:** Parallel force calculations
  - **Data Layout:** Memory access optimization
  - **Newton 3:** Force calculation optimization



Linked Cells | Verlet Cluster Lists | Verlet Lists

Simpler Memory Access
Lower Memory Overhead

Fewer redundant calculations

[Newcome et al., 2024]

Structure of AutoPas

- Three main areas:
  - 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

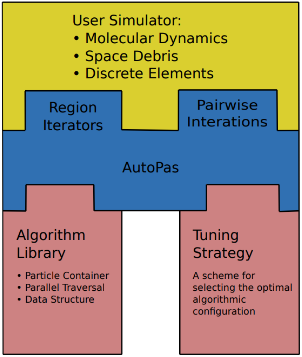
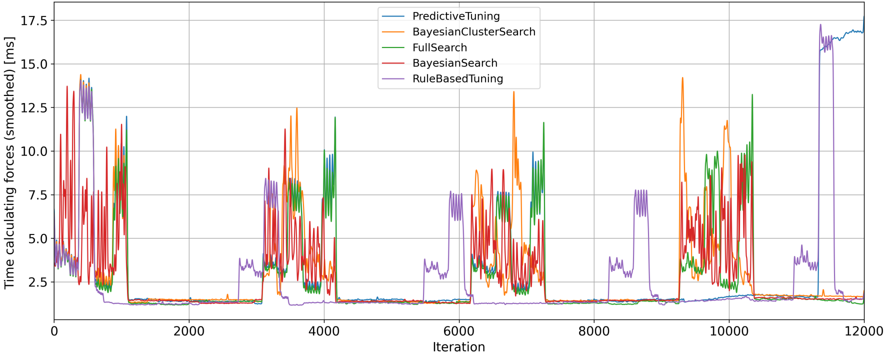


Figure: [Newcome et al., 2023]

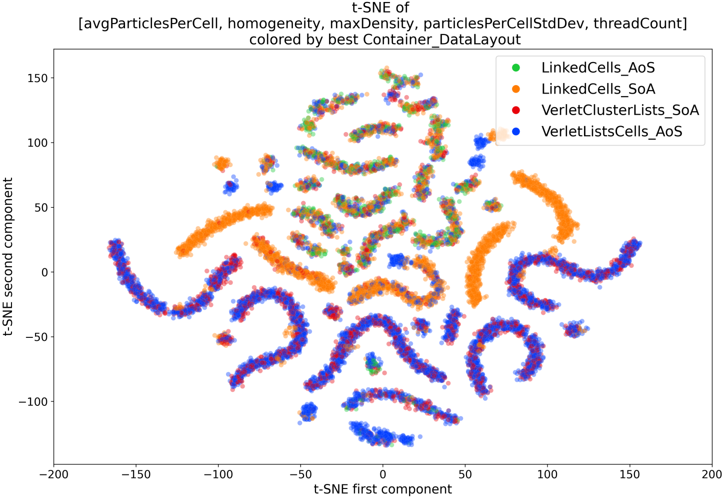
[1] Container $\times$ Traversal $\times$ Data Layout $\times$ Newton 3 $\times$ Load Estimator $\times$ Cell Size Factor

Auto-Tuning

- Tuning Phase → Simulation Phase → Repeat
- Potential Tuning Overhead



Idea: Tuning based on Simulation State



Fuzzy Logic System

- (Fuzzy) Rule-based system
- Human-like reasoning to model systems $f : \mathbb{R}^n \to \mathbb{R}$
- Linguistic terms instead of numerical values
  - What is *hot*? What is *cold*?
  - Allow smooth transitions between terms

Example (Heater Control)

Input: temperature (e.g. 20°C), humidity (e.g. 60%)

Output: heater power (e.g. 50%)

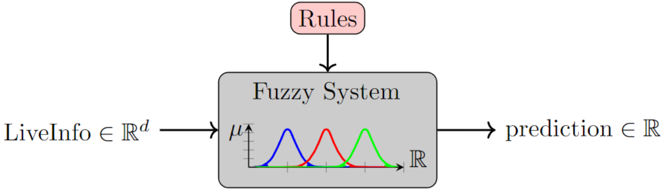
Rules:

IF temp is *cold*	**AND**	humidity is *dry*	**THEN** power is *high*
IF temp is *hot*	**OR**	humidity is *wet*	**THEN** power is *low*
IF temp is *warm*			**THEN** power is *medium*

Table of Contents

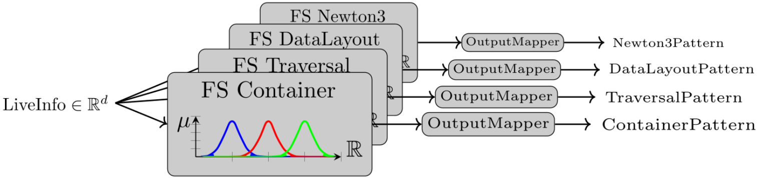
Challenge 1: Numerical Output

- Fuzzy Tuning not directly applicable to AutoPas
  - Tuning is an *algorithm selection* problem
  - Fuzzy tuning provides functions $f : \mathbb{R}^n \to \mathbb{R}$
  - Big Question: How to interpret the numerical output?



Approach 1: Component Tuning

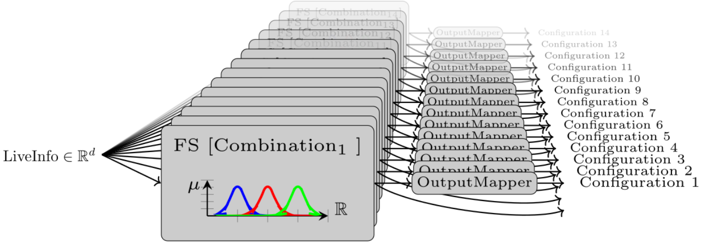
- Explicit Fuzzy System for each tunable parameter
  - Continuous representation of the parameter values



- Example: **IF** avgParticlesPerCell is *low* **AND** threadCount is *low*
  THEN traversal is *vcl_c06*

Approach 2: Suitability Tuning

- A Fuzzy System for **each** possible configuration
- Predict *suitability* of each configuration



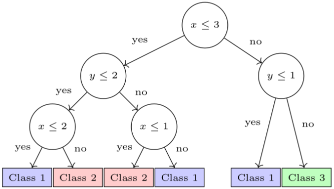
- Example: **IF** threadCount is *high* **AND** avgParticlesPerCell is *low*
  THEN suitability_LinkedCells_AoS_lc_c18_disabled is *bad*

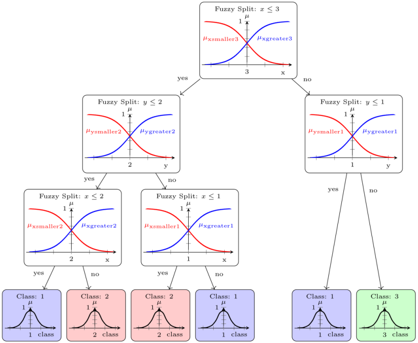
Challenge 2: Expert Knowledge

- How to design the Fuzzy System?
  - Creating it manually?
    - ✗ Requires extensive expert knowledge
    - ✗ Difficult to formalize non-trivial knowledge
  - Extracting rules from data?
    - ✓ No prior expert knowledge required
    - ✓ Semi-automated process

Data-Driven Rule Extraction

- Machine learning to generate rules [Crockett et al., 2006]
  1. Train Decision Tree on the data
  2. Decision Tree → Fuzzy Decision Tree
  3. Fuzzy Decision Tree → Fuzzy Rules





Fuzzy Decision Trees → Fuzzy Rules

- *Unnest* the fuzzy decision tree

Rule	Antecedent	Consequent
1	x *is* smaller3 $\wedge$ y *is* smaller2 $\wedge$ x *is* smaller2	*class is* 1
2	x *is* smaller3 $\wedge$ y *is* smaller2 $\wedge$ x *is* greater2	*class is* 2
3	x *is* smaller3 $\wedge$ y *is* greater2 $\wedge$ x *is* smaller1	*class is* 2
4	x *is* smaller3 $\wedge$ y *is* greater2 $\wedge$ x *is* greater1	*class is* 1
5	x *is* greater3 $\wedge$ y *is* smaller1	*class is* 1
6	x *is* greater3 $\wedge$ y *is* greater1	*class is* 3

Fuzzy Rule Extraction for `md_flexible`

- Collect dataset of `md_flexible` simulations
- For each tuning phase *i*, store:
  - LiveInfoData: `maxDensity, homogeneity, threadCount, ...`
  - TuningData: `Container, Traversal, Newton3, ...,` **`Time`**
- Introduce *relative speed* metric
  - Absolute time is not meaningful

$$\text{relative speed}_{config}^{(i)} = \frac{\mathrm{t}_{best}^{(i)}}{\mathrm{t}_{\mathrm{config}}^{(i)}}$$

Resulting Dataset

- Contains expected *relative speed* based on:
  - Simulation state
  - Configuration

ParticlesPerCell			Miscellaneous			Configuration			
avg	max	stddev	homo-genity	max-density	threads	Container DataLayout	Traversal	Newton3	Relative Speed
0.905	23	0.0129	0.0354	0.531	1	LinkedCells_AoS	lc_sliced	enabled	0.450641
2.201	13	0.0144	0.0861	0.627	24	VerletListsCells_AoS	vlc_sliced	disabled	0.594117
0.905	18	0.0136	0.0431	0.319	4	LinkedCells_AoS	lc_sliced_c02	enabled	0.454632
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Fuzzy Rule Extraction

Antecedent				Consequent
avgParticlesPC	**homogeneity**	**particlesPCStdDev**	**threadCount**	**Traversal**
lower than 1.553	higher than 0.047	lower than 0.023	higher than 2.5	"lc_sliced, vlc_c18, lc_sliced_c02"
	lower than 0.037	lower than 0.023	lower than 26.0	"vcl_c06, vlc_c18, vlc_sliced_c02"
⋮	⋮	⋮	⋮	⋮

Example: Component Tuning Rules

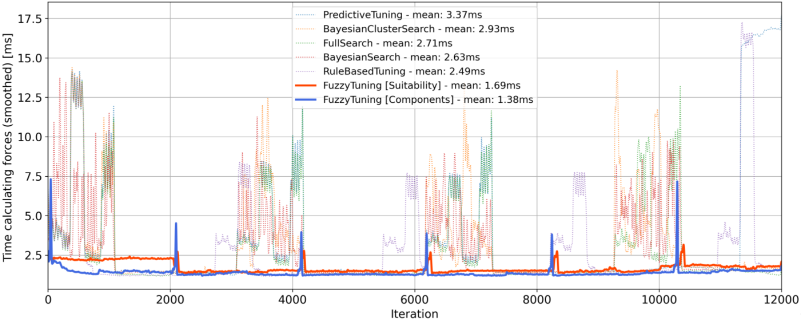
Antecedent				Consequent
avgParticlesPC	**homogeneity**	**particlesPCStdDev**	**threadCount**	**Suitability LinkedCells_AoS lc_c01_disabled**
	lower than 0.084	higher than 0.029	higher than 26.0	"medium"
	higher than 0.084	higher than 0.029	higher than 26.0	"bad"
		higher than 0.02	lower than 2.5	"poor"
⋮	⋮	⋮	⋮	⋮

Example: Suitability Tuning Rules

Table of Contents

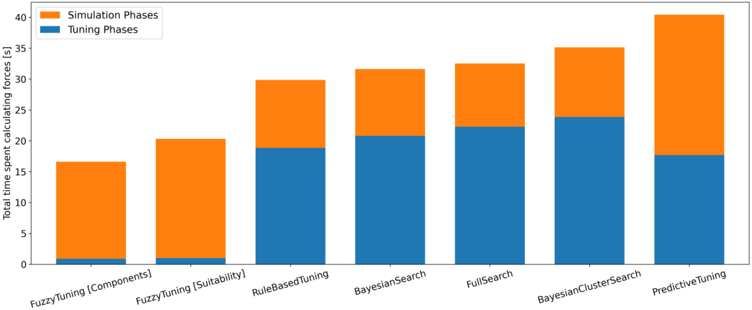
Benchmark 1: Exploding Liquid

- Fuzzy Tuning Approaches:
  - Very short tuning phases
  - Selected configurations perform well
  - Winning configurations are (mostly) equivalent



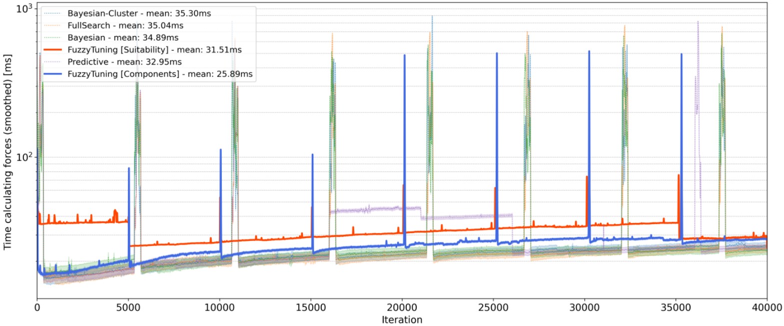
Total Time: Exploding Liquid

- Fuzzy Tuning is good because:
  - Few evaluated configurations
  - Good evaluated configurations
- Massive reduction in time spent tuning



Benchmark 2: Spinodal Decomposition (MPI)

- Component approach performs well
- Suitability approach misses the optimal configuration
  - However: no tuning overhead
  - Can this make up for the suboptimal configurations?



Total Time: Spinodal Decomposition

- Component tuning wins again
- Suitability tuning:
  - Fast tuning phases compensate for suboptimal configurations!
  - Improvement: Encourage longer tuning phases
    - Increase suitability threshold (Top 10% → Top 30%)

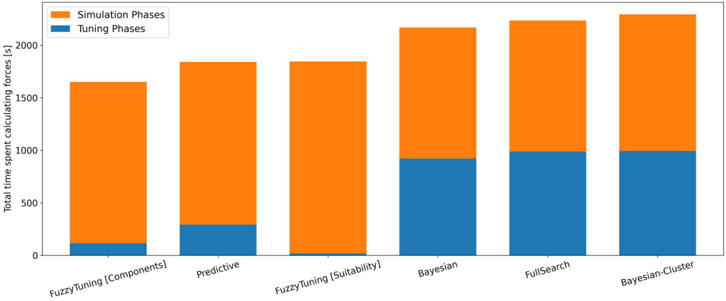


Table of Contents

Conclusion

- Fuzzy Tuning is very promising for AutoPas
  - Massive reduction in tuning overhead
  - Reduction of total simulation time (up to factor 1.96x)
  - Among the best tuning strategies (but very complex)
- Ongoing Challenge:
  - Rule generation
    - ✗ Requires a lot of data (1.1GB)
    - ✗ Unappealing for users
    - ✗ No universal solution (showed some generalization)

Conclusion

- Fuzzy Tuning is very promising for AutoPas
  - Massive reduction in tuning overhead
  - Reduction of total simulation time (up to factor 1.96x)
  - Among the best tuning strategies (but very complex)
- Ongoing Challenge:
  - Rule generation
    - ✗ Requires a lot of data (1.1GB)
    - ✗ Unappealing for users
    - ✗ No universal solution (showed some generalization)

Improvement Ideas

- Dynamic Rule Generation
  - Update expert knowledge on the fly
  - Automatically adapt to new scenarios
- Improvements to the Tuning Process
  - Investigate *early stopping* mechanism
  - Dismiss slow configurations early
  - Solve tuning overhead once and for all?
- Simplification of the Model
  - Ensemble of Decision Trees instead of Fuzzy Systems
  - Maybe comparable results?

Thank you for your attention!

Questions?

References I

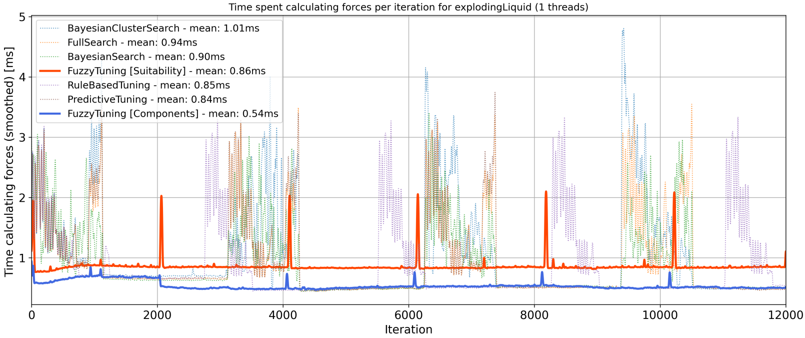
Crockett, K., Bandar, Z., Mclean, D., and OShea, J. (2006).
On constructing a fuzzy inference framework using crisp decision trees.
Fuzzy Sets and Systems, 157(21):2809–2832.

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.
In *SIAM Conference on Parallel Processing (PP24)*. SIAM.

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

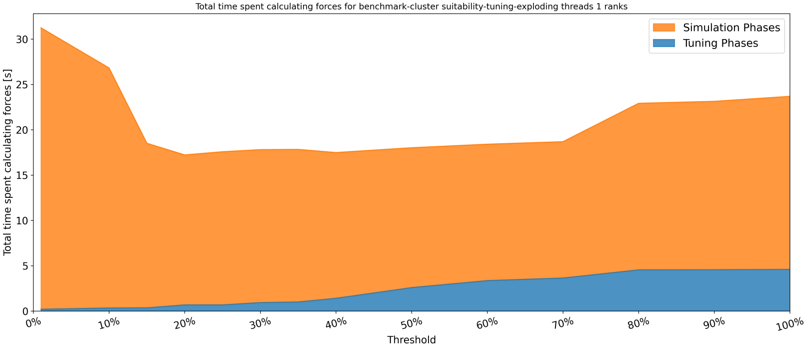
Backup: What happens on new scenarios?

- Exploding Liquid: bigger $\varepsilon \rightarrow$ more spacing
- Component Tuning is winning again

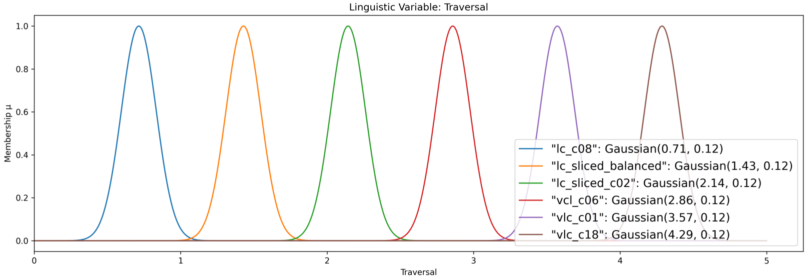


Backup: Optimal Suitability Threshold

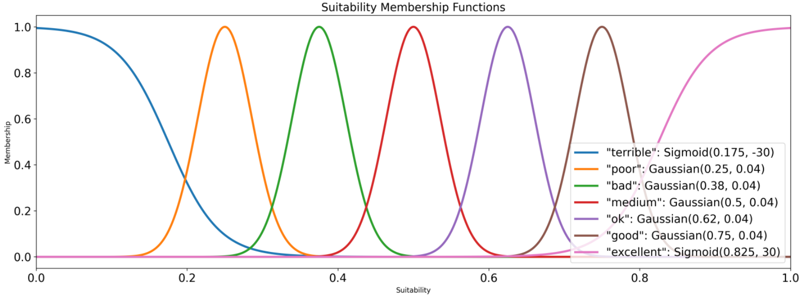
- Goal: find optimal hyperparameters for suitability-approach



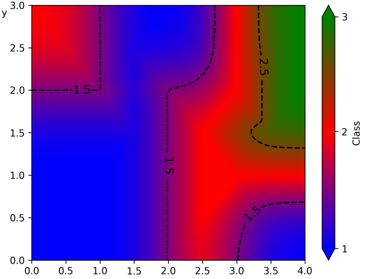
Backup: Linguistic Variables for Component Tuning



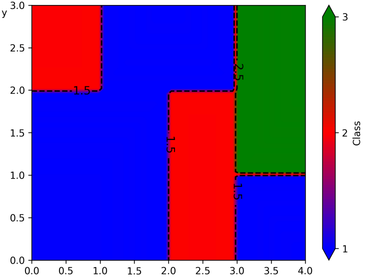
Backup: Linguistic Variables for Suitability Tuning



Backup: Decision Surfaces



(a) Center of Gravity - Defuzzification

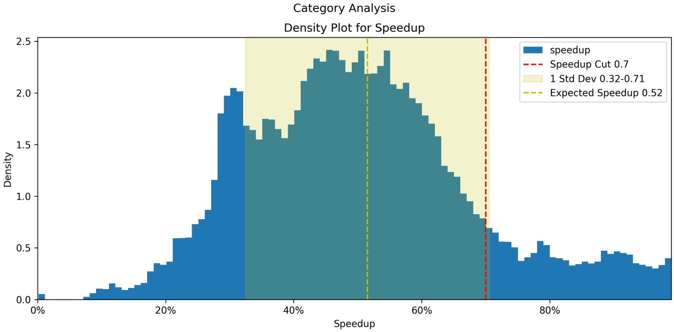


(b) Mean of Maxima - Defuzzification

Figure: Decision Surfaces of Fuzzy System

Backup: Speedup Distribution

- How good is the average configuration?



Backup: Quality of Predictions

- How well do tuning strategies suggest good configurations?

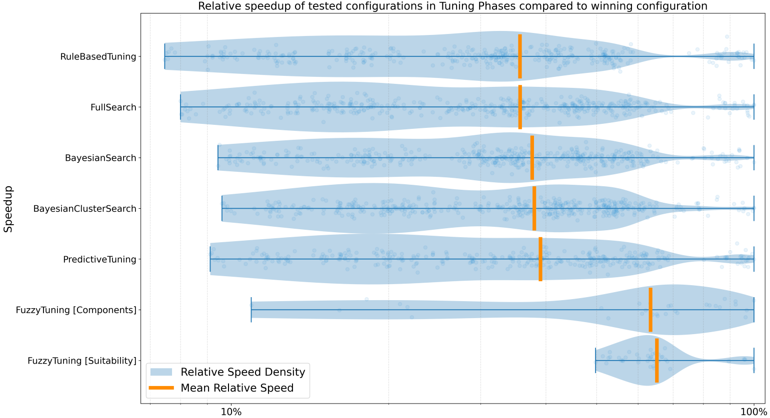


Figure: Source: MathWorks - Fuzzy Inference Process