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Bachelor Thesis Final Presentation

Exploring Fuzzy Tuning Technique for Molecular Dynamics Simulations in AutoPas

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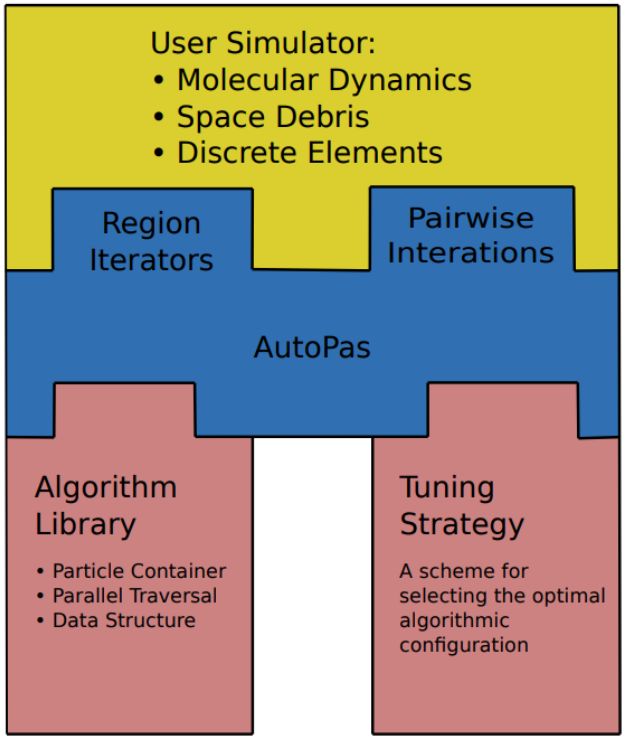
AutoPas

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

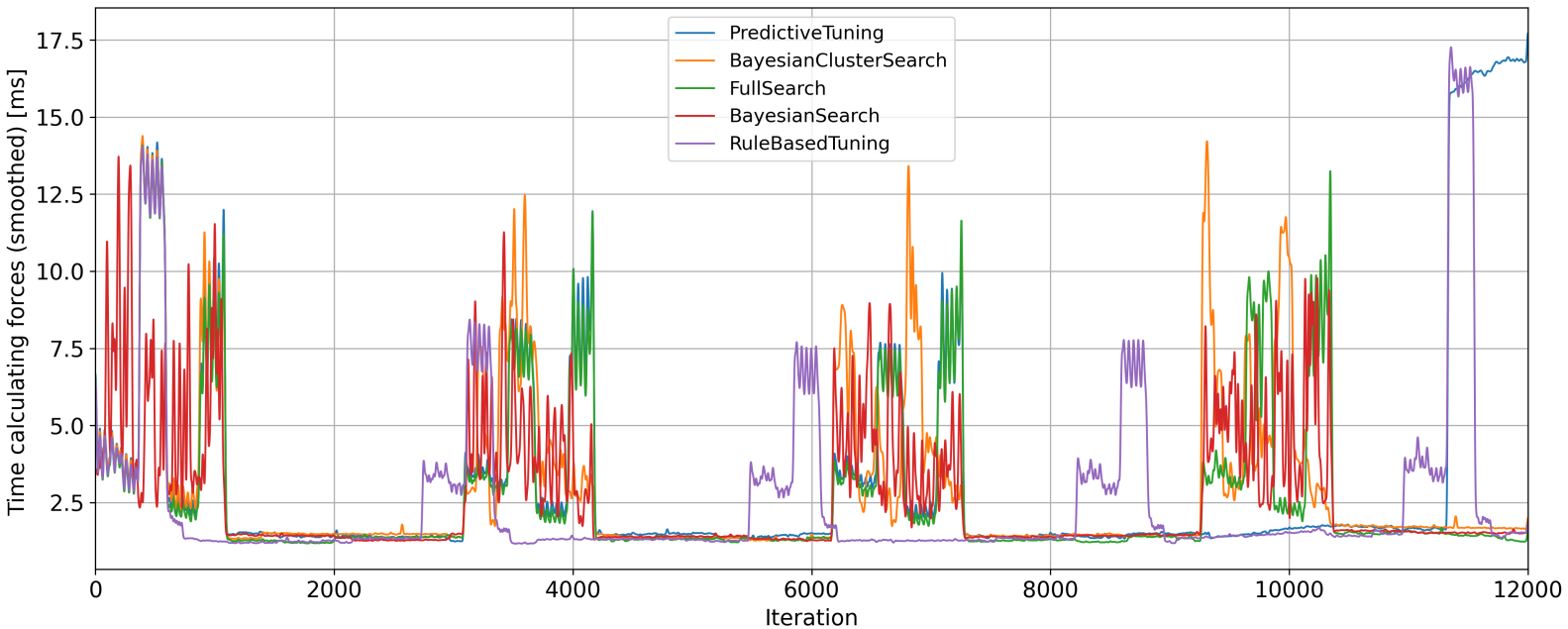


Source: [Newcome et al., 2023]

[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
  - Expensive, Time consuming
- Simulation Phase: Use the best configuration



Fuzzy Logic Systems

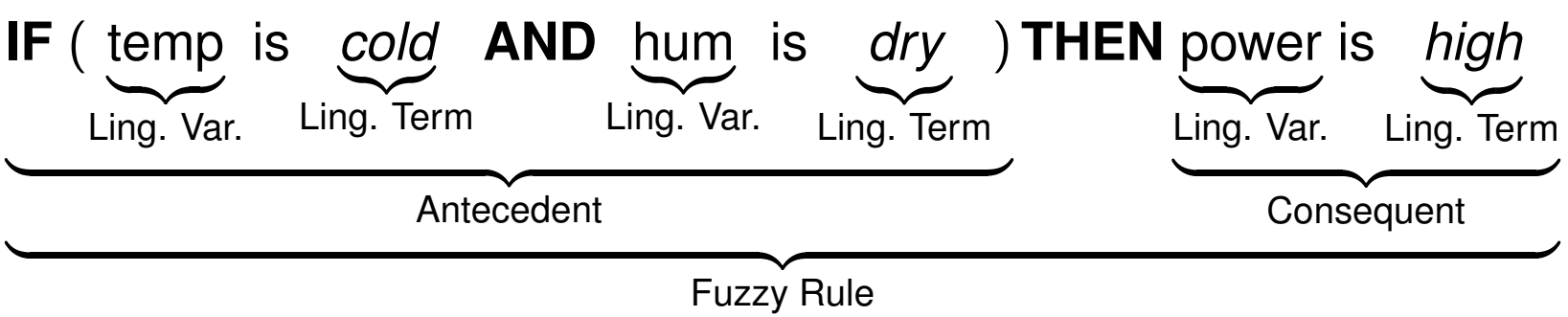
- Use human-like reasoning to model complex systems
- Example: Heater Control
  - Input: temperature (e.g. 20°C), humidity (e.g. 50%)
  - Output: heater power (e.g. 50%)
  - Rules:

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*

- Very easy to understand and interpret
- Can handle uncertainty and imprecise information
- Complexity is abstracted away in the linguistic terms (e.g. *cold, warm, hot*)
- Black box $f : \mathbb{R}^n \to \mathbb{R}$

Mathematical Foundations

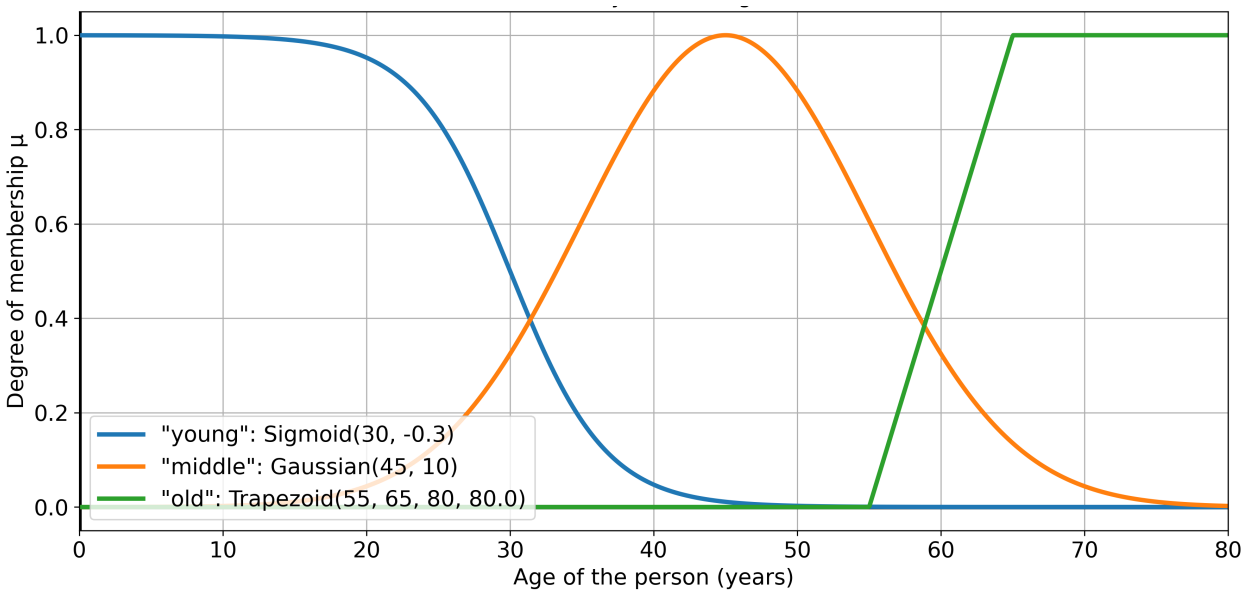
- Consider the Fuzzy Rule:



- Fuzzy Logic Systems consist of:
  - Linguistic Terms / Fuzzy Sets (e.g. *cold, warm, hot*)
  - Linguistic Variables (e.g. temperature, humidity, power)
  - Fuzzy Logic Operators (e.g. **AND, OR, NOT**)
  - Fuzzy Rules (e.g. **IF** *antecedent* **THEN** *consequent*)

Fuzzy Sets

- Fuzzy Sets are generalizations of classical sets
  - Classical Sets: binary membership function $\in_A$: $A \to \{false, true\}$
- Fuzzy Sets are defined by:
  - Underlying Crisp Set X (e.g. $age \subset \mathbb{R}$)
  - **Continuous** membership function $\mu_{\tilde{A}} : X \to [0, 1]$
- Allow for uncertainty. When is a person young?



Linguistic Variables

- Linguistic Variables can take on linguistic terms / fuzzy sets
  - E.g. *age* can take *young*, *middle-aged* or *old*
- Instead of using crisp values (35 years), we use a combination of linguistic terms to describe the age (Fuzzyification):

$$35 \text{ years} \implies \begin{cases} 20\% \text{ young} \\ 60\% \text{ middle-aged} \\ 0\% \text{ old} \end{cases}$$

- Each fuzzy set describes a *collection* of crisp values
- This allows for very human-like rules.
  - E.g. **IF** age is *young* **THEN** fitness is *high*
  - Internally ”age is *young*” represents the associated fuzzy set

Fuzzy Logic Operators

- Fuzzy Logic Operators are used to modify/combine fuzzy sets
- Extension of boolean logic operators to real numbers
  - $\wedge : \{false, true\} \times \{false, true\} \rightarrow \{false, true\}$
  - **AND** : $[0, 1] \times [0, 1] \rightarrow [0, 1]$
- Extended operators need to maintain the classical semantics
- Typically, Fuzzy Logic Operators are defined as:
  - **AND:** Corresponds to the intersection of fuzzy sets

$$\mu_{\tilde{A} \cap \tilde{B}}(x) = \min(\mu_{\tilde{A}}(x), \mu_{\tilde{B}}(x))$$

  - **OR:** Corresponds to the union of fuzzy sets

$$\mu_{\tilde{A} \cup \tilde{B}}(x) = \max(\mu_{\tilde{A}}(x), \mu_{\tilde{B}}(x))$$

  - **NOT:** Corresponds to the complement of a fuzzy set

$$\mu_{\neg \tilde{A}}(x) = 1 - \mu_{\tilde{A}}(x)$$

Arbitrary Complex Fuzzy Sets

- With the above operators, we can define arbitrary complex fuzzy sets:
- TODO insert tree from thesis

Fuzzy Rules

- Each rule is of the form: **IF** *antecedent* **THEN** *consequent*
  - Both antecedent and consequent are fuzzy sets
  - E.g. **IF** age is *young* **THEN** fitness is *high*
- The output $\tilde{R}$ of a rule is a fuzzy set
  - Rules are applied with the Mamdani Implication:
  - $\mu_{\tilde{R}}(x) = \min(\mu_{\tilde{A}}(x), \mu_{\tilde{B}}(x))$
  - *Effect* of the rule is limited by the *strength* of the antecedent
- A Fuzzy System can consist of multiple rules acting on the same linguistic variable
  - The total *effect* on the output is the combination/union of all individual rule outputs

Defuzzification

- Process of converting arbitrary fuzzy sets to a crisp value
  - Special case: Fuzzy set created from Linguistic Variable age

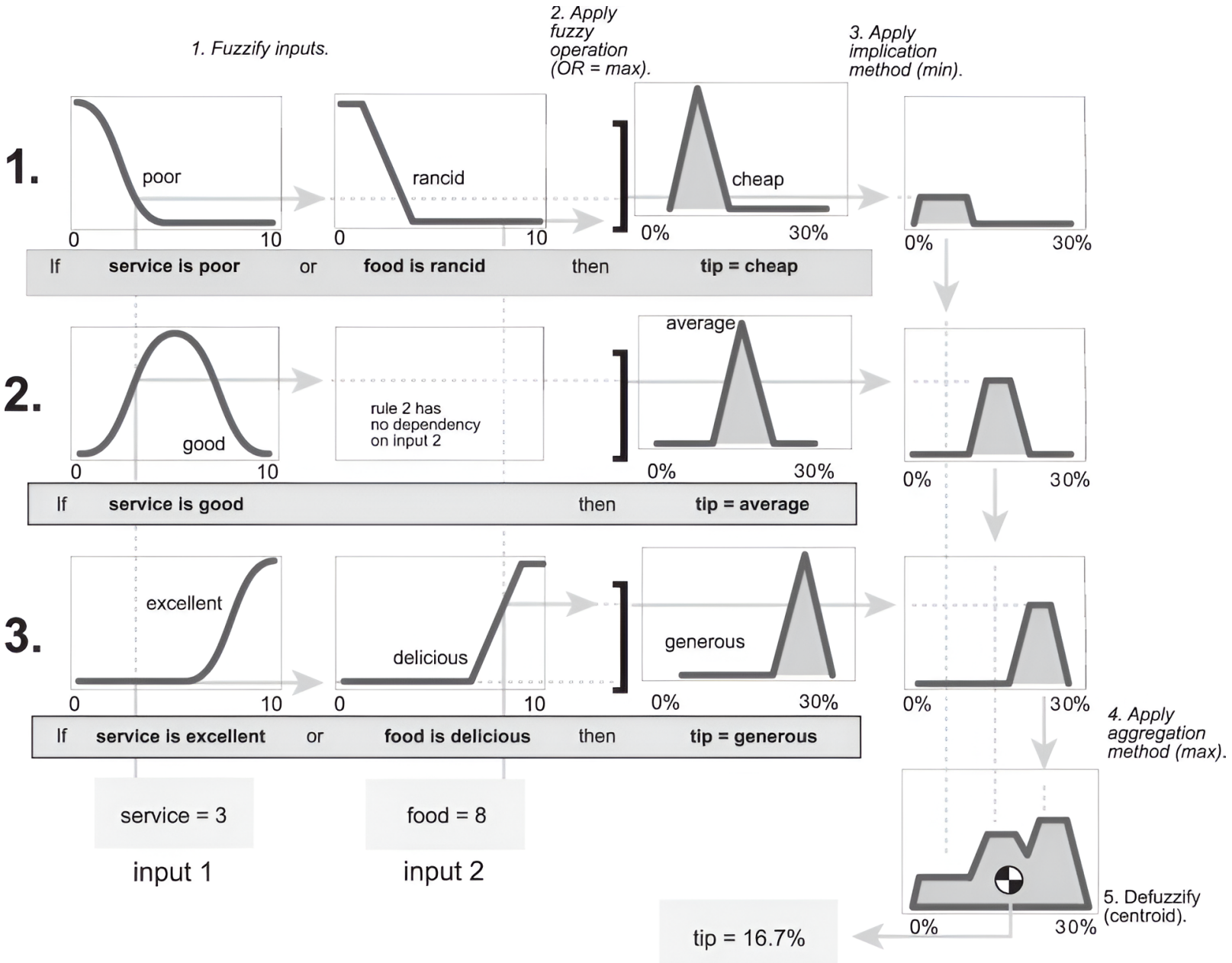
$$\begin{cases} 20\% \text{ young} \\ 60\% \text{ middle-aged} \\ 0\% \text{ old} \end{cases} \Longrightarrow 35 \text{ years}$$

- Common methods:
  - **Centroid:** Weighted average of the output fuzzy set

$$\text{Centroid} = \frac{\int x \cdot \mu_{\tilde{R}}(x) dx}{\int \mu_{\tilde{R}}(x) dx}$$

  - **Mean of Maxima:** Average of the maximum values of the output fuzzy set
- Core idea: Represent certain aspects of the fuzzy set as a crisp value

Source: MathWorks - Fuzzy Inference Process



- TODO: Maybe add decision surfaces here

Fuzzy Tuning Strategy

- Main Idea: Use Fuzzy Logic to tune AutoPas
- Benefits:
  - Similar to Rule-Based Tuning
  - Potentially more expressive and powerful
  - Still easy to understand and interpret
- Challenges and Questions for AutoPas:
  - How to perform tuning? (Fuzzy System : $f : \mathbb{R}^n \rightarrow \mathbb{R}$)
  - What are the input variables?
  - What are the output variables?
  - How to create the fuzzy rules? Expert knowledge?
  - How to specify the linguistic terms / fuzzy sets?

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.