



SCHOOL OF COMPUTATION, INFORMATION
AND TECHNOLOGY

DER TECHNISCHEN UNIVERSITÄT MÜNCHEN

Bachelor's Thesis in Informatics

**Exploring Fuzzy Tuning Technique for
Molecular Dynamics Simulations in
AutoPas**

Manuel Lerchner



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Untersuchung von Fuzzy Tuning Verfahren für Molekulardynamik-Simulationen in AutoPas

Author: Manuel Lerchner
Supervisor: Univ.-Prof. Dr. Hans-Joachim Bungartz
Advisors: Manish Kumar Mishra, M.Sc. &
Samuel Newcome, M.Sc.
Date: 10.08.2024

I confirm that this bachelor's thesis is my own work and I have documented all sources and material used.

Munich, 10.08.2024

Manuel Lerchner

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3 Implementation

This chapter describes the implementation of the Fuzzy Tuning technique in AutoPas. The implementation is divided into three main parts: the generic Fuzzy Tuning framework, the Tuning Strategy, and the Rule Parser. The Fuzzy Tuning framework is the core of this implementation and implements the mathematical foundation of this technique. The Tuning Strategy is the interface between the Fuzzy Tuning framework and the AutoPas simulation. It is responsible for interacting with AutoPas and updating the queue of configurations. The Rule Parser is responsible for parsing the rule base supplied by the user and converting it into the internal representation used by the Fuzzy Tuning framework. The implementation of the Fuzzy Tuning technique in AutoPas is designed to be as generic as possible to allow for easy integration of new types of rule bases.

3.1 Fuzzy Tuning Framework

The Fuzzy Tuning framework implements the mathematical foundation of the Fuzzy Tuning technique. It consists of several components that work together to apply the Fuzzy Rules to the input variables and generate the output variables. The components of the Fuzzy Tuning framework are as follows:

- **Crisp Set:** The Crisp Set is used to model k-cells used as the underlying sets over which the Fuzzy Sets are defined. A k-cell is a hyperrectangle in the k-dimensional space constructed from the Cartesian product of k intervals $I = I_1 \times I_2 \times \dots \times I_k$ where $I_i = [x_{low}, x_{high}] \subset \mathbb{R}$ is an interval in the real numbers. They are used to define the underlying sets over which the corresponding fuzzy set is defined and can be thought of as the parameter space of the input variable.
- **Fuzzy Set:** A fuzzy set consists of a membership function that assigns a degree of membership to each element of the Crisp Set. There are two types of membership functions: The `BaseMembershipFunction` and the `CompositeMembershipFunction`. The `BaseMembershipFunction` implement a function $f : \mathbb{R} \rightarrow [0, 1]$ that directly maps the crisp value to the degree of membership. The `CompositeMembershipFunction` is used to create new fuzzy sets by recursively combining existing fuzzy sets and their membership functions with generic functions. This helps to split up the complex fuzzy sets of the rule base into smaller, more manageable parts. Lets say we have a fuzzy set \tilde{A} defined over the Crisp Set X and a fuzzy set \tilde{B} defined over the Crisp Set Y . Both membership functions are functions mapping the respective Crisp Set to the degree of membership ($\mu_{\tilde{A}} : X \rightarrow [0, 1]$ and $\mu_{\tilde{B}} : Y \rightarrow [0, 1]$). Since both membership functions directly map the Crisp Set to the degree of membership, they are considered `BaseMembershipFunctions`. When we want to create a new fuzzy set $\tilde{C} = \tilde{A} \cap \tilde{B}$ this new fuzzy set is defined over the Crisp Set $X \times Y$ and thus needs to provide a

add chapter

membership function $\mu_{\tilde{C}} : X \times Y \rightarrow [0, 1]$. As described in this membership function is defined as $\mu_{\tilde{C}}(x, y) = \min(\mu_{\tilde{A}}(x), \mu_{\tilde{B}}(y))$, which can be thought of as recursively combining the membership functions of \tilde{A} and \tilde{B} with the minimum function.

This way of combining fuzzy sets builds a tree structure where the leafs calculate a direct membership value and the inner nodes combine the membership values of their children and pass them up to their parent.

add image

- **Linguistic Variable:** A linguistic variable is a variable whose values are terms in a natural language. Each term is associated with a fuzzy set that defines its concept using the language of fuzzy logic. The linguistic variables can then be used to express rules in a human-readable way.
- **Fuzzy Rule:** A fuzzy rule is a conditional statement that describes the relationship between input- and output variables. It consists of an antecedent and a consequent both of which are fuzzy sets. During the evaluation of the rule, the antecedent is evaluated to determine the degree to which the rule is satisfied and thus the effect of the rule can be reduced accordingly.
- **Fuzzy Control System:** The Fuzzy Control System combines all the concepts described above to create a system that can evaluate a set of fuzzy rules and generate an output based on the input variables. Such a control system acts like a black box $f : \mathbb{R}^n \rightarrow \mathbb{R}$ that takes a set of crisp input variables and returns the predicted value.

Add UML Diagram

3.2 Rule Parser

The Rule Parser is responsible for parsing the rule base supplied by the user and converting it into the internal representation used by the Fuzzy Tuning framework. It makes use of the ANTLR4¹ parser generator to create a parser for a domain-specific language tailored to the needs of the Fuzzy Tuning. The language is inspired by common standards such as the Fuzzy Control Language (FCL)² but is more lightweight and also allows for the connection of the Fuzzy Tuning framework to the AutoPas simulation. The transformation of the parsed rules into the internal representation is done by a visitor pattern that traverses the parse tree generated by ANTLR4 and internally builds the corresponding objects of the Fuzzy Tuning framework.

Appart from the obvious grammar rules for the fuzzy sets and rules, the language encompasses a few additional constructs to allow for the connection to the AutoPas simulation. This is a crucial part of the tuning framework as the continuous outputs of the Fuzzy Control Systems need to be mapped to the discrete configuration space of the AutoPas simulation. We chose a approach inspired by Mohammed et al. [MKEC22]'s work on scheduling algorithms and used a ranking system that embeds all available configurations in the continuous output space of the Fuzzy Control System. The Tuning Strategy then selects the configuration closest to the predicted value.

chose other example

For a linguistic variable *Container DataLayout* such a mapping could look like this:

¹<https://www.antlr.org/>

²<https://www.fuzzylite.com/>

OutputMapping:

```
"Container_DataLayout":
  0.666 => [container="LinkedCells", dataLayout="SoA"],
           [container="VerletClusterLists", dataLayout="SoA"],
           [container="VerletListsCells", dataLayout="AoS"]
  1.333 => [container="LinkedCells", dataLayout="SoA"],
           [container="VerletClusterLists", dataLayout="SoA"],
           [container="VerletListsCells", dataLayout="AoS"],
           [container="VerletListsCells", dataLayout="SoA"]
  2.0    => [container="LinkedCells", dataLayout="SoA"],
           [container="VerletClusterLists", dataLayout="SoA"],
           [container="VerletListsCells", dataLayout="AoS"],
           [container="VerletListsCells", dataLayout="SoA"],
           [container="VerletLists", dataLayout="SoA"]
  2.666 => [container="VerletClusterLists", dataLayout="SoA"],
           [container="VerletListsCells", dataLayout="AoS"]
  3.333 => [container="VerletClusterLists", dataLayout="SoA"],
           [container="VerletListsCells", dataLayout="AoS"],
           [container="VerletListsCells", dataLayout="SoA"]
```

This mapping states that AutoPas should prefer all configurations matching one of the patterns `[container="VerletClusterLists", dataLayout="SoA"]` and `[container="VerletListsCells", dataLayout="AoS"]` if the output of the Fuzzy Control System is close to 2.666.

Add example image

The full grammar specification can be found in Listing A.1.

3.3 Tuning Strategy

The Tuning Strategy implements the interface between the Fuzzy Tuning framework and the AutoPas simulation. It is responsible for interacting with AutoPas and updating the queue of configurations.

It does this by evaluating all Fuzzy Systems present in the rule file with the current LiveInformation of the simulation. The LiveInformation is a snapshot of the current state of the simulation and contains summary statistics about various aspects of the simulation. This evaluation yields a list of all configurations selected by the Fuzzy Control Systems and those replace the current queue of configurations which need to be tested.

Currently two different modes of interpreting the rules are implemented:

Suitability Approach

Individual Tuning Approach

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Bibliography

- [BMK96] Bernadette Bouchon-Meunier and Vladik Kreinovich. Axiomatic description of implication leads to a classical formula with logical modifiers: (in particular, mamdani’s choice of ”and” as implication is not so weird after all). 1996.
- [CBMO06] Keeley Crockett, Zuhair Bandar, David Mclean, and James O’Shea. On constructing a fuzzy inference framework using crisp decision trees. *Fuzzy Sets and Systems*, 157(21):2809–2832, 2006.
- [GSBN21] Fabio Alexander Gratl, Steffen Seckler, Hans-Joachim Bungartz, and Philipp Neumann. N ways to simulate short-range particle systems: Automated algorithm selection with the node-level library autopas. *Computer Physics Communications*, 273:108262, 2021.
- [GST⁺19] Fabio Alexander Gratl, Steffen Seckler, Nikola Tchipev, Hans-Joachim Bungartz, and Philipp Neumann. Autopas: Auto-tuning for particle simulations. In *2019 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW)*, pages 748–757, 2019.
- [LM15] Benedict Leimkuhler and Charles Matthews. *Molecular Dynamics: With Deterministic and Stochastic Numerical Methods*. Interdisciplinary Applied Mathematics. Springer, May 2015.
- [MKEC22] Ali Mohammed, Jonas H. Müller Korndörfer, Ahmed Eleliemy, and Florina M. Ciorba. Automated scheduling algorithm selection and chunk parameter calculation in openmp. *IEEE Transactions on Parallel and Distributed Systems*, 33(12):4383–4394, 2022.
- [Mur12] Kevin P. Murphy. *Machine Learning: A Probabilistic Perspective*. The MIT Press, 2012.
- [SGH⁺21] Steffen Seckler, Fabio Gratl, Matthias Heinen, Jadran Vrabec, Hans-Joachim Bungartz, and Philipp Neumann. Autopas in ls1 mardyn: Massively parallel particle simulations with node-level auto-tuning. *Journal of Computational Science*, 50:101296, 2021.
- [VBC08] G. Viccione, V. Bovolin, and E. Pugliese Carratelli. Defining and optimizing algorithms for neighbouring particle identification in sph fluid simulations. *International Journal for Numerical Methods in Fluids*, 58(6):625–638, 2008.