

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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Exploring Fuzzy Tuning Technique for Molecular Dynamics Simulations in AutoPas

Untersuchung von Fuzzy Tuning Verfahren für Molekulardynamik-Simulationen in AutoPas

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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

Acknowledgements

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Abstract

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Zusammenfassung

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Part I.

Introduction and Background

1. Introduction

Write some useful intro. Here are tips along the way:

1.1. Tips

1.1.1. How to Describe

When listing several points you have three basic options:

- | | | |
|---------------|----------------|--|
| • itemize | 1. itemize | itemize short, unordered |
| • enumerate | 2. enumerate | enumerate short ordered |
| • description | 3. description | description listing of descriptions. Also nice for longer ones. |

1.1.2. How to Quote

”This is a quote!”

- Citations to a source can be made like this `\cite{grat117task}` = [Gra17]
Always join text and the citation with a non-breaking space: `text~\cite{foo}`.
- Referencing Sections, Figures, Tables, Formulas: `\autoref{sec:intro}` = Chapter 1.
- Footnotes for url or further notes: `\footnote{\url{https://www.top500.org}}` ¹

1.1.3. How to Math

Use the align environment for equations especially if you want to align them somehow.

$$1 + 1 \neq 3 \tag{1.1}$$

$$\left(\frac{10}{1}\right) - 9 = 1 \tag{1.2}$$

¹<https://www.top500.org>

1.2. Environments

1.2.1. How to Figure

Anything can also be put in multiple columns.

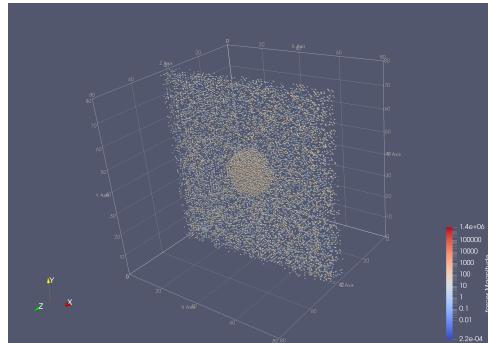


Figure 1.1.: Some Caption. Always also include a source if it wasn't created by you!
Source: [Gra17]

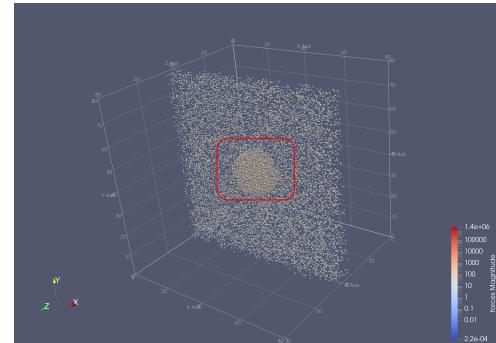


Figure 1.2.: Figures can be drawn on or completely generated with tikz.

Subfigures If grouping of several pictures seems reasonable, think about using subfigures. This often comes in handy with plots.

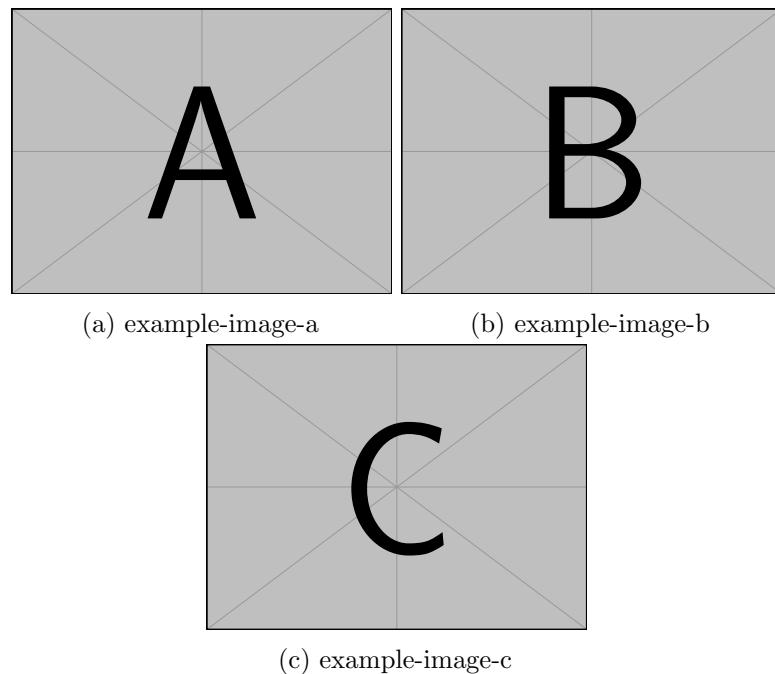


Figure 1.3.: One caption to describe them all.

1.2.2. How to Algorithm

Algorithm 1: Bogosort

Input: data array
Output: data sorted

// Checks if array is sorted

1 **Function** is_sorted(*data*):
2 **for** *i* \leftarrow 0 **to** *data.size()* - 1 **do**
3 **if** *data*[*i*] > *data*[*i*+1] **then**
4 **return** false
5 **return** true

// actual algorithm

6 **Function** bogosort(*data*):
7 **while** not is_sorted(*data*) **do**
8 random.shuffle(*data*)

Figure 1.4.: some description what is happening

1.2.3. How to Code

```
1 void runner(int type, void *data){  
2     switch(type)  
3     {  
4         case taskType1:  
5             // do stuff using data  
6         case taskType2:  
7             // do other stuff using data  
    }
```

Listing 1.1: General form of a typical runner() function.

1.2.4. How to Table

| | | |
|----------|---|------------------------|
| bla left | bla centered over two lines | bla right |
| bla left | bla centered cell spanning two columns | cell spanning two rows |

Table 1.1.: Fancy table that can contain line breaks and extended cells.

Part II.

Appendix

A. Some more stuff

For everything that does not really belong in the thesis but is good to mention.

List of Figures

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Bibliography

[Gra17] Fabio Alexander Gratl. Task based parallelization of the fast multipole method implementation of ls1-mardyn via quicksched. Master's thesis, Institut für Informatik 5, Technische Universität München, Garching, November 2017.