d|b|t|a

Fachgebiet
Dynamik und Betrieb technischer Anlagen

This Is a Very Good Title That Illustrates What This Great Piece of Work Is All About and That Gives an Impression of What a Long Title Looks Like

Wissenschaftliche Arbeit zur Erlangung des Grades
Master of Science (M.Sc.)

vorgelegt von
First name second name

Matrikelnummer
XXXXXX

Unter der wissenschaftlichen Leitung von
Prof. Dr.-Ing. habil. Jens-Uwe Repke

Unter der wissenschaftlichen Betreuung von
My advisor, M.Sc.

Berlin, Januar 2019

Technische Universität Berlin
Fakultät III – Prozesswissenschaften
Institut für Prozess- und Verfahrenstechnik
Fachgebiet Dynamik und Betrieb technischer Anlagen

Eidesstattliche Erklärung

Hiermit erkläre ich an Eides statt, dass ich die vorliegende Arbeit selbstständig und eigenhändig sowie ausschließlich unter Verwendung der aufgeführten Quellen und Hilfsmittel angefertigt habe.

First name second name
Berlin, 30. Januar 2019

I hereby confirm that I prepared this thesis independently and by exclusive reliance on literature or tools indicated herein.

First name second name
Berlin, 30th January, 2019

Danksagung

Ein paar nette Worte / Some nice words...

Zusammenfassung

Deutsch

Dies hier ist ein Blindtext zum Testen von Textausgaben. Wer diesen Text liest, ist selbst schuld. Der Text gibt lediglich den Grauwert der Schrift an. Ist das wirklich so? Ist es gleichgültig, ob ich schreibe: „Dies ist ein Blindtext“ oder „Huardest gefburn“? Kjift – mitnichten! Ein Blindtext bietet mir wichtige Informationen. An ihm messe ich die Lesbarkeit einer Schrift, ihre Anmutung, wie harmonisch die Figuren zueinander stehen und prüfe, wie breit oder schmal sie läuft. Ein Blindtext sollte möglichst viele verschiedene Buchstaben enthalten und in der Originalsprache gesetzt sein. Er muss keinen Sinn ergeben, sollte aber lesbar sein. Fremdsprachige Texte wie „Lorem ipsum“ dienen nicht dem eigentlichen Zweck, da sie eine falsche Anmutung vermitteln. Dies hier ist ein Blindtext zum Testen von Textausgaben. Wer diesen Text liest, ist selbst schuld. Der Text gibt lediglich den Grauwert der Schrift an. Ist das wirklich so? Ist es gleichgültig, ob ich schreibe: „Dies ist ein Blindtext“ oder „Huardest gefburn“? Kjift – mitnichten! Ein Blindtext bietet mir wichtige Informationen. An ihm messe ich die Lesbarkeit einer Schrift, ihre Anmutung, wie harmonisch die Figuren zueinander stehen und prüfe, wie breit oder schmal sie läuft. Ein Blindtext sollte möglichst viele verschiedene Buchstaben enthalten und in der Originalsprache gesetzt sein. Er muss keinen Sinn ergeben, sollte aber lesbar sein. Fremdsprachige Texte wie „Lorem ipsum“ dienen nicht dem eigentlichen Zweck, da sie eine falsche Anmutung vermitteln.

Schlüsselwörter: *Keyword1; Keyword2; Keyword3*

English

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

Keywords: *Keyword1; Keyword2; Keyword3*

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Symbolverzeichnis

Konstanten

Symbol	Beschreibung	Einheit
R	Universelle Gaskonstante = 8,314 46	$\mathrm{J\,mol^{-1}\,K^{-1}}$

Dimensionslose Kennzahlen

Symbol	Beschreibung	Definition
Re	Reynoldszahl	$\frac{wd\rho}{\eta}$

Griechische Symbole

Symbol	Beschreibung	Einheit
α	Non-randomness factor in NRTL-Modell	–
α	Parameter in Gleichung für Verdampfungsenthalpie	$\mathrm{J\,mol^{-1}}$
α	Trennfaktor für binäre VLEs	–
Δ	Differenz	verschieden

Indizes

Symbol	Beschreibung
i	Index für Komponenten
j	Index für Komponenten
k	Index der Strukturgruppe

Lateinische Symbole

Symbol	Beschreibung	Einheit
A	Parameter in Antoine-Gleichung	–
A	Porter-Parameter	–
B	Parameter in Antoine-Gleichung	K
B	Zweiter Virialkoeffizient (Leiden-Form)	$\mathrm{m^3\,mol^{-1}}$
B'	Zweiter Virialkoeffizient (Berlin-Form)	$\mathrm{Pa^{-1}}$

Operatoren

Symbol	Beschreibung	Definition
∇	Nabla-Operator	$\left[\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n}\right]^T$
rot	Rotationsoperator	$\mathrm{rot}\ \vec{g} = \nabla \times \vec{g}$

Superskripte

Symbol	Beschreibung
E	Exzess
III	Phase/Zustand 3
II	Phase/Zustand 2
I	Phase/Zustand 1

Subskripte

Symbol	Beschreibung
0	Reinstoff
0	zu Beginn der Reaktion
c	Kritisch

Abkürzungsverzeichnis

ab	**A**ctive **b**ounds
DAE	**D**ifferential-**a**lgebraic **e**quation (system)
SUNDIALS	**Su**ite of **n**onlinear and **di**fferential-**al**gebraic equation **s**olvers

1 Guidelines

This chapter introduces the guidelines for writing a thesis at the Process Dynamics and Operations Group. It is recommended to use LaTeX as the code of this style guide can directly be used for the thesis. However, a Word version of this template is also available. In the template, the correct fonts, font sizes, citation style, etc. are already set.

1.1 Most Important Style Specifications for LaTeX and Word

The most important style specifications are:

- page format: A4, double page, justification, 11 pt for standard font size;
- line spacing:
  - Word: 1.5;
  - LaTeX: linespacing is set with the `setspace` package any may not be changed;
- fonts :
  - Word: Palatino Linotype (text) and MS Reference Sans Serif (headings);
  - LaTeX: the font types are specified within this template and may not be changed;

- margins:
  - Word: 35 mm (top), 60 mm (bottom), 27 mm (inside), 40 mm (outside);
    binding correction: 15 mm (only possible when double page is selected); exception: front page;
  - LaTeX: the given settings for BCOR and DIV may not be changed;
- maximum number of pages (only content, excluding lists of ... and appendix): 80 pages (bachelor thesis), 100 pages (master thesis);
- the layout of the front page is fixed and must not be changed, neither in LaTeX nor in Word;
- of course, loading additional packages in LaTeX for functionality is fine.

Attention: If these specifications are (partially) ignored, it will have an impact on the evaluation.

1.2 First Steps

1. **carefully read this whole chapter**
2. set the language of the document in the a_Packages.tex file with the `babel` package. You will notice that this text is written in English while certain headings are in German. This is because the `babel` package is currently loaded with ngerman as default language (see Abschn. 1.7).
3. change the necessary entries in c_Meta.tex (e.g. your name, matriculation number, etc.), set the right value of the `isDiss` variable and the `isMT` variable (if it is a thesis) in this file
4. check whether biblatex and makeindex were set up correctly (see Abschn. 1.8.1)
5. check whether you can compile this document without errors (this should always be the case as long as all necessary packages are in-

stalled). This template was successfully compiled with a TEXLive 2017 distribution. **Some problems appeared when users did not have the newest versions of the used packages in this template. If you run into trouble, please update all your packages**[1]. See some more instructions for TEXLive and MiKTEX in Abschn. 1.8.3

6. remove the guidelines chapter from this document by deleting it and removing it from the 0_Text.tex file in the folder 03_Content
7. add your own .bib file for your references or use the present one (it is recommended to simply use the given one)
8. start writing your thesis - good luck!
9. note that not all of the shown items in the following sections *must* be part of your thesis. If a certain aspect does not apply to you, e.g. a List of Algorithms, just remove it from the thesis.

1.3 General Information

a) the current „Prüfungsordnung“ overrides the following rules if they contradict the „Prüfungsordnung“.

b) a thesis is a scientific-technical documentation that must satisfy requirements regarding structure and form. It should be precisely formulated and well-written, i.e. no orthographic or grammar mistakes, etc.

c) the thesis should be logically structured.

d) the thesis should present its scientific-technical content while remaining comprehensible. Hence, the author should repeatedly put him- or herself into the position of the reader and evaluate the thesis in this regard.

e) the Figure, i.e. picture, diagram, photo, is preferred to long explanations.

[1] https://tex.stackexchange.com/questions/55437/how-do-i-update-my-tex-distribution, January 2019

f) results must be tractable. Hence, the applied methods, assumptions, boundary conditions, experiments, and computer codes must be pointed out and explained in sufficient detail.

g) calculations should be documented. This is of course difficult for large models. In this case, the code should be attached to the printed or digital appendix.

h) the thesis should focus on the central themes and aspects. Other information should be referenced appropriately, but does not have to be repeated extensively.

1.4 Form

a) the thesis must be written in German or English.

b) sentences should be comprehensible. Germans tend to formulate complex phrases with many sub-clauses. This should be avoided.

c) physical units must always be given and are preferably stated in SI units. Units must not be stated in brackets:

   – *WRONG:* Pressure P [Pa];

   – *RIGHT:* Pressure P in Pa.

   The only correct use of square brackets is shown here for the voltage: [U] = V, i.e. the unit of the voltage is volt.

d) a List of Symbols and a List of Abbreviations must be included. This is done with the `nomentbl` and the `acronym` package in this template. Furthermore, symbols should be explained in the text after their first appearance. A List of Algorithms or other lists can be added if necessary.

e) figures, tables, and equations must be numerated and referenced in the text. This is automatically done using the `caption` package (see Abschn. 1.10) and the `\autoref` command (Abschn. 1.10.7). For example, a Figure is named Figure chapter.Num (Fig. 2.1). The numeration

is done automatically in this template. In addition, figures and tables must also be explained and discussed in the text.

f) figures should be chosen to support comprehension. In particular, the most important details and relevant labels must be *readable*.

g) extensive tables or figures that are repeatedly referenced in the text should be put in the appendix.

h) information or data not generated by the author must always be referenced. Citations/references are used to

   – document and justify one's own statements,

   – differ between one's own statements and those made by others,

   – help the reader to assess the origin of a statement

   All information not generated by the author must be marked with a short reference, which is accompanied by the extensive reference in the bibliography. It is not important if this information appears directly or indirectly in the text. We either use the authoryear or the numerical short citation.
   The most important rule is: The references must be complete and follow a consistent format. This is more important than following a specific citation style. If possible, the DOI/ISBN of an article/book should be part of the citation. This is also included automatically in this template. The commands and some examples are shown in Abschn. 1.10.4.

1.5 Appearence

a) the format of the page numbering is already specified and may not be changed.

b) there is a maximum of four indenture levels in the text and a maximum of three levels in the table of contents.

c) the sections of the appendix are numerated alphabetically in capital Latin letters. This is already specified in this template.

d) important aspects can be emphasized with *italics*, **bold writing**, or using the *emphasize command* `\emph`. Underlining words should be avoided.

e) paragraphs should not start in the last two lines of a page („Schusterjunge“ or orphen) or end in the first two lines of a page („Hurenkind“ or widow). This is automatically achieved with the `nowidow` package in this template.

1.6 Template Structure

This section describes the structure of this template. Questions remaining unanswered can be forwarded to Christian Hoffmann (c.hoffmann@tu-berlin.de).

1.6.1 Features

- valid for theses or dissertations
- can be used with online editors, such as Overleaf (see Abschn. 1.9.2)
- can be used in German and English
- simple generation of List of Symbols (Latin, Greek, etc.) with the `nomentbl` package
- simple generation of List of Abbreviations with the `acronym` package
- includes bibliography via biblatex and biber
- includes DOI/ISBN/URL automatically in references

1.6.2 Main Document

- is called main.tex
- this document must be compiled in LaTeX

1.6.3 00_Arara_and_Latexindent

The following files are located in this folder:

a) indent.yaml
   - contains the rule for arara 3.0A
   - more information can be found in Anhang D

b) localSettings.yaml
   - contains the local settings for automatic indenting
   - more information can be found in Abschn. 1.9.3 and Anhang D

1.6.4 01_Document_administration

The following files are located in this folder:

a) a_Packages.tex
   - contains all packages, which are loaded
   - packags are sorted based on their application
   - all packages of this template and their references are stated in Tab. E.1

b) b_Commands.tex
   - contains further commands regarding formatting and look of the document
   - also sorted

c) c_Meta.tex
   - contains meta information regarding author, etc.
   - contains a boolean variable to select whether it is a dissertation or a bachelor/master thesis
   - contains a boolean variable to select whether it is a master or a bachelor thesis

d) d_NomenclatureCommands.tex
   - defines structure of the List of Symbols
   - optional argument defines the class of a symbol (Latin, Greek, ...)
   - makeindex is used for the generation of the List of Symbols. A short instruction how to run makeindex correctly in Texmaker is given in Abschn. 1.8.1.

e) e_Header_Footer.tex
   - defines headers and footers

f) f_CodeLanguageSpecifications
   - can be used to define a set of keywords and comment commands for a certain programming language
   - if you want to apprehend your code in your thesis, you can either copy the code to an lstlistings environment (see examples in Anhang A and Anhang B) or directly include your files
   - more information can be found in the lstlistings documentation

1.6.5 02_Prematter

The following files are located in this folder:

a) a_Cover_Diss.tex and a_Cover_Thesis.tex
   - creates the cover page
   - main.tex loads either a_Cover_Thesis.tex (cover of a bachelor/-master thesis) or a_Cover_Diss.tex (cover of a dissertation), depending on the value of `isDiss` set in c_Meta.tex. Both covers are shown in Abb. 1.1.

b) b_Declaration.tex
   - declaration that the thesis was written honestly

c) c_Acknowledgements.tex

- thank important people

d) d_Summary.tex

- summarize your thesis in German and English

e) e_Nomenclature.tex

- enter all symbols and explain them
- examples are provided

f) f_Abbreviations.tex

- enter all abbreviations and explain them
- examples are provided

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aus Berlin

von der Fakultät III – Prozesswissenschaften
der Technischen Universität Berlin
zur Erlangung des akademischen Grades

Doktor der Ingenieurswissenschaften
- Dr.-Ing. -

genehmigte Dissertation

Promotionsausschuss:

Vorsitzende: Prof. Dr.-Ing. habil. Martina Superwichtig
1. Gutachter: Prof. Dr.-Ing. habil. Jens-Uwe Repke
2. Gutachter: Prof. Dr.-Ing. Hans-Georg Wichtig

Tag der wissenschaftlichen Aussprache: 20. Dezember 2018

Berlin, 2019

(a) *Cover in diss. mode (isDiss=true).*

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Unter der wissenschaftlichen Betreuung von
My advisor, M.Sc.

Berlin, Januar 2019

Technische Universität Berlin
Fakultät III – Prozesswissenschaften
Institut für Prozess- und Verfahrenstechnik
Fachgebiet Dynamik und Betrieb technischer Anlagen

(b) *Cover in thesis mode (isDiss=false).*

Abb. 1.1: *Covers of this template.*

1.6.6 02a_Dissertation_files

This folder contains files that are only needed for dissertations. They are included if `isDiss` is set to `true`. Bachelor/Master theses do not have to consider them. However, if you want to dedicate your thesis to someone, you can of course include the dedication. The following files are located in this folder:

a) a_Dedication.tex
   - dedicate your dissertation to someone

b) b_Publications.tex
   - states all publications that were written in preparation of the dissertation

1.6.7 03_Content

The following files are located in this folder:

a) 0_Text.tex
   - loads all chapters

b) X_iii.tex
   - contains the single chapters
   - can be split further if deemed necessary

1.6.8 04_Literature

The following files are located in this folder:

a) Bibliography.bib
   - contains the literature

1.6.9 05_Appendix

The following files are located in this folder:

a) 0_Appendix.tex
   - loads all appendix chapters

b) X_Appendix.tex
   - contains the Xth appendix

1.7 Language: English or German?

The language of this document is set with the `babel` package. The order of the loaded languages determines the default language. Usually, `ngerman` is default (and hence the *second*) language. The `babel` package automatically sets the localized names for Tables and Figures, provides the correct hyphenation, and does more language-related things. In case the thesis is written in English, the order of the languages when loading the `babel` package must be changed.
If the language is English, it is recommended to change the output decimal marker for SI units (`siunitx` package) to a period. This can be changed in the a_Packages.tex file where the `siunitx` package is loaded.

1.8 LaTeX Editor Settings and Maintenance

1.8.1 Biblatex and Makeindex

- to compile the file correctly, biblatex and makeindex are used
- command line for setting up biblatex in Texmaker (see Abb. 1.2):
  a) Windows:
     `"C:/path_to/biber.exe" %`
     in TeXLive, biber is located in `bin/win32`

b) Linux:
`"/usr/path_to/biber" %`

c) MacOS:
`"/usr/path_to/biber" %.bcf`

– command line for setting up makeindex in Texmaker (see Abb. 1.2):

a) Windows:
`"C:/path_to/makeindex.exe" %.nlo -s mynomentbl.ist -o %.nls`
in TEXLive, makeindex is located in `bin/win32`

b) Linux:
`"/usr/path_to/makeindex" %.nlo -s mynomentbl.ist -o %.nls`

c) MacOS:
`"/usr/path_to/makeindex" %.nlo -s mynomentbl.ist -o %.nls`

– the necessary mynomentbl.ist file is located in the template folder

– if you use another editor than Texmaker, check your editor's documentation to find out how to run biblatex (biber) and makeindex in this software. However, the paths/commands should be the same.

1.8.2 Compiling the Document

The following commands/scripts must be run to compile the document completely:

1. pdflatex: This generates a first PDF. At this point, the List of References and the List of Symbols are missing.
2. biblatex: Run biber (Texmaker standard short key: F11) after you set it up according to Abschn. 1.8.1. This creates the necessary temporary reference file.
3. makeindex: Run makeindex (Texmaker standard short key: F12) after you set it up according to Abschn. 1.8.1. This creates the necessary temporary nomenclature file.

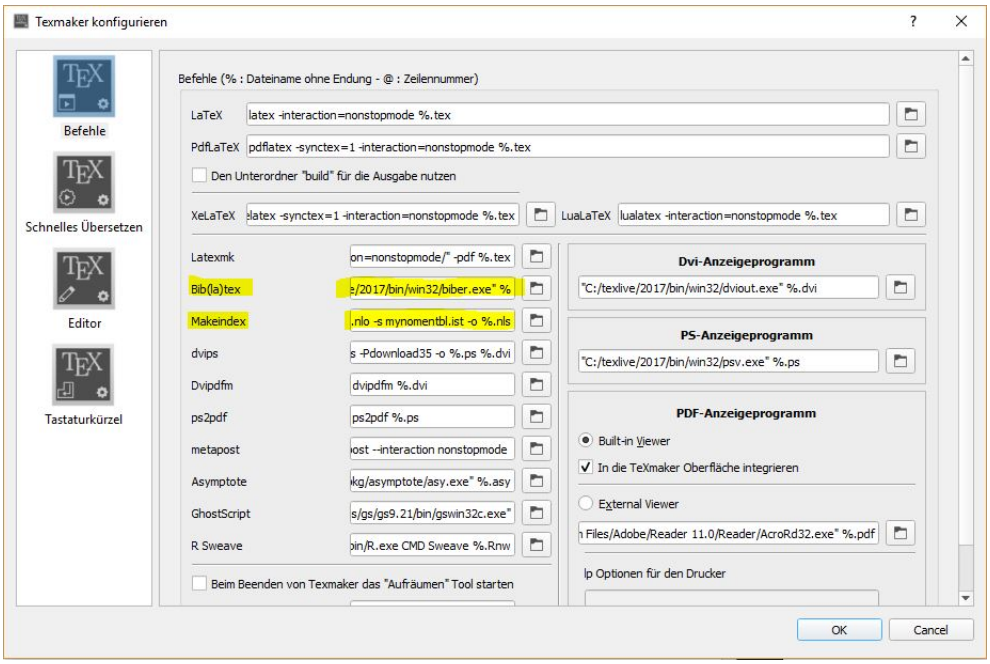


Abb. 1.2: *Setting up biblatex and makeindex in Texmaker. Zoom in if you need more details.*

4. pdflatex (two times): The first run should already generate the List of References and the List of Symbols. The second run should update all citations etc. in the PDF.

1.8.3 Updating Packages in TeXLive and MiKTeX

As stated above, compiling problems appeared with this template when old versions of the packages were used. Unfortunately, there does not seem to be a possibility to automatically check for updates of packages when they are included in a LaTeX document.
In case you have issues when compiling this document, start with updating all your packages. The following instructions are valid for a Windows operating system.

TeXLive: In TeXLive, the packages are managed via the tlmgr. The GUI of the tlmgr is located in `texlive/year/bin/win32`. In this folder, you find

a file called tlmgr-gui.exe. Execute this file and the application shown in Abb. 1.3 starts. Use this application to update your packages.

MiKTEX: In MiKTEX, the packages are managed in the MiKTEX console (package manager in older versions), see Abb. 1.4. Use this application to update your packages.

Similar applications are available on all other operating systems. Restart your LATEX editor after updating all packages and see whether you can compile this template without errors. If your problem persists, contact Christian Hoffmann (c.hoffmann@tu-berlin.de).

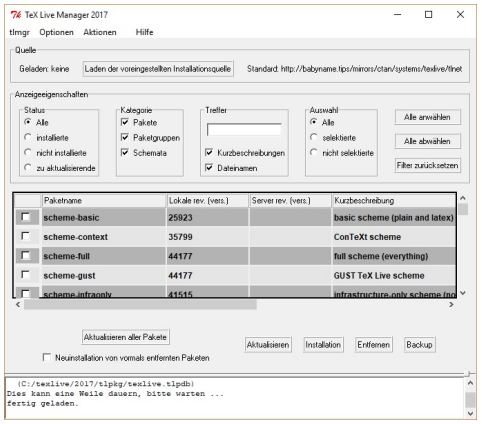


Abb. 1.3: *Updating packages in Windows for TEXLive.*

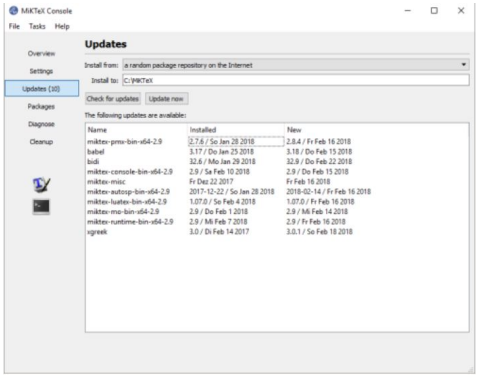


Abb. 1.4: *Updating packages in Windows for MiKTEX.*

1.9 Extra Features

The following sections introduce a few extra features. None of them are necessary for a thesis, but they might be of use for some people.

1.9.1 Compatibility with PDF/A

Dissertations are stored as PDF/A at the university library. To ensure compatibility of this template with PDF/A, the `pdfx` package is used with the

option a-1b. The compiled PDF was successfully validated with Callas[2], as recommended by the university library[3]. Note that contrary to the descriptions given in the linked document in Fußnote 3, a specific color profile is *not* necessary if you use an up-to-date version of the `pdfx` package as it automatically includes a free color profile. Check the documentation of the `pdfx` package to find how to include other color profiles. Normally, the default should however suffice.

1.9.2 Support for Overleaf or other online editors

This template was successfully tested with Overleaf, an online editor for LaTeX documents[4], see Abb. 1.5. If you would like to write in such an online environment, simply upload the template folder to a new empty project and compile it online. In this way, you do not have to install any LaTeX distribution locally. **Note that this is not advised if you have sensitive data, e.g. from a company in the industry. In this case, your data should remain on your computer!**
The only dependency Overleaf does not directly support is `nomentbl`. As this package needs makeindex, you have to tell the Overleaf compiler how to proceed. This information is contained in the latexmkrc file in this template folder. Simply upload the latexmkrc file to the Overleaf project next to main.tex and Overleaf should compile this file correctly. In some cases, you may first have to clear the cache to remove old temporary files[5].

1.9.3 Automatic Indenting of .tex Files

Indenting *can* be used for structuring one's document, e.g. by indenting everything within an equation environment, but is certainly *not* a must-have for a thesis. If you do not need automatic indenting, you can skip this section.

[2] https://conversion.ub.tu-berlin.de/, December 2018
[3] https://www.ub.tu-berlin.de/fileadmin/pdf/Verlag/UV_pdfaDE.pdf, December 2018
[4] https://de.overleaf.com/, January 2019
[5] https://www.overleaf.com/learn/how-to/Clearing_the_cache, January 2019

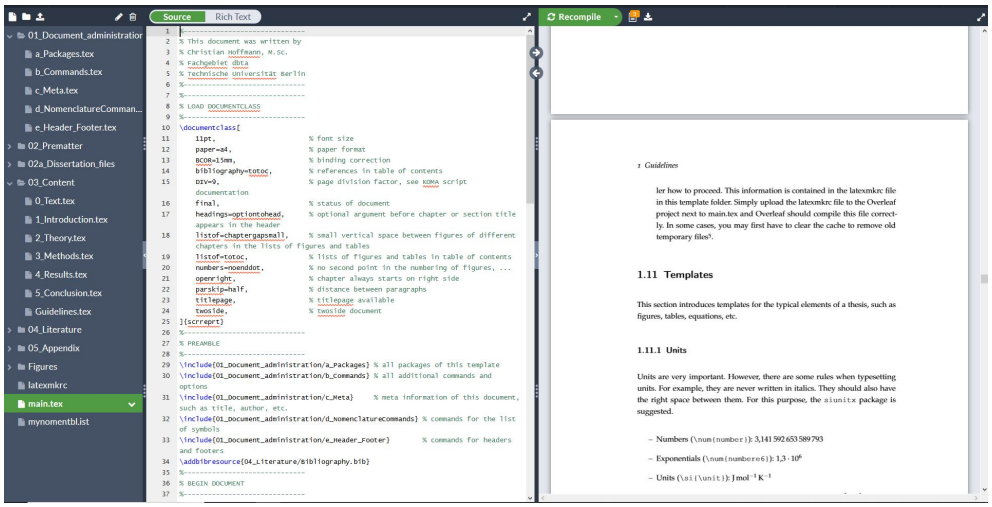


Abb. 1.5: *Template on Overleaf.*

Unfortunately, LaTeX does not offer automatic indenting as do, for example, Matlab or Python. However, the perl script-based `latexindent` can be used for automatic indenting of the source code. This executable is part of every LaTeX distribution. There are two ways of using `latexindent`: directly running `latexindent` or calling it via `arara`[6]. Only the first option is described here for a Windows operating system (the instructions for Linux and Mac should be similar; only the file extension .exe is propably different). The second option is described in Anhang D.
To get automatic indenting, add a user command in Texmaker (User → User Commands → Edit User Commands). You might call one menu item `latexindent`. The command should be

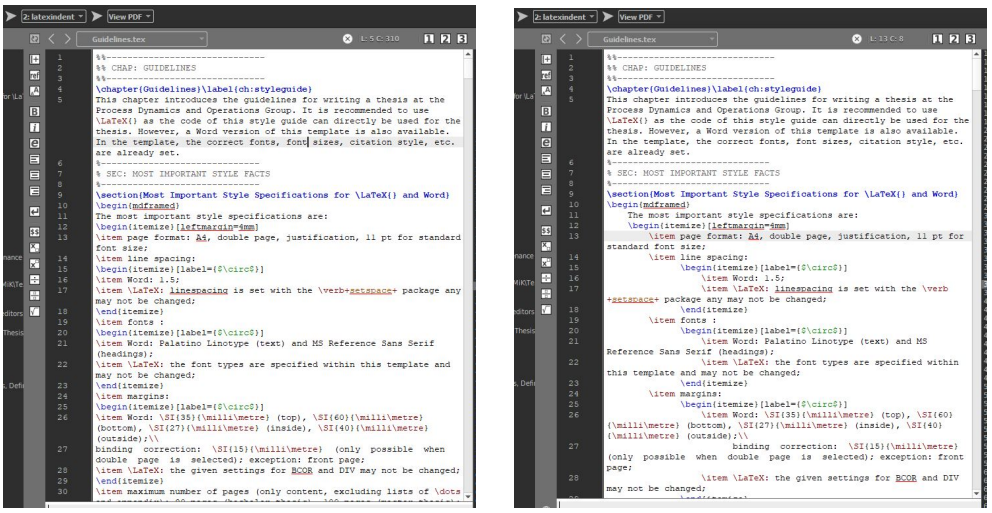
```
C:/path_to_texlive/year/bin/win32/latexindent.exe -w %.tex -l="
    absolute_path_to_thesis_template/Thesis_template/
    LaTeX_template_thesis/00_Arara_and_Latexindent/localSettings.
    yaml"
```

Code 1.1: *Setting up latexindent in Texmaker.*

This means that `latexindent` is executed with writing rights (-w) on the current .tex file with local settings (-l) in the given path. These local settings

[6] https://tex.stackexchange.com/questions/126241/autoindent-in-texmaker, January 2019

are the only issue, because the absolute path can of course change if you move your folder. However, the relative path would always change depending on which file you actually want to indent.
The local settings are important as they specify that only one backup is created. For more information, please refer to the documentation of latexindent.
You can then execute your user new command in Texmaker with the opened file in question. Afterwards. update your file by clicking on File → Reload document from file. The result is shown in Abb. 1.6. **Note that automatic indenting might not be available for online editors.**



(a) *Before.* ***(b)*** *After.*

Abb. 1.6: *Before (left) and after (right) automatic indenting with latexindent.*

1.10 Templates for Typical Elements of a Thesis

This section introduces templates for the typical elements of a thesis, such as figures, tables, equations, etc.

1.10.1 Units

Units are very important. However, there are some rules when typesetting units. For example, they are never written in italics. They should also have the right space between them. For this purpose, the `siunitx` package is suggested.

- numbers (`\num{number}`): 3,141 592 653 589 793
- exponentials (`\num{numbere6}`): $1{,}3 \cdot 10^6$
- units (`\si{\unit}`): $\mathrm{J\,mol^{-1}\,K^{-1}}$
- numbers+units (`\SI{number}{\unit}`): $8{,}314\,\mathrm{J\,mol^{-1}\,K^{-1}}$
- ranges (`\SIrange{number1}{number2}{\unit}`): 4 to 10 K.
- uncertainty (`\num{number(uncertainty)}`): $410{,}33 \pm 0{,}55$
- uncertainty with units (`\SI{number(uncertainty)}{\unit}`): $(410{,}33 \pm 0{,}55)\,\mathrm{J}$

1.10.2 Figures

A template for a Figure is given in Abb. 1.7. Abbildung 1.7 should not be abbreviated at the beginning of a sentence. Note that the often used `\ref` command is not used here. Instead, Abschn. 1.10.7 introduces the `\autoref` command. In addition, a short command for including figures was set up with the `xparse` package:

```
\myfigure[opt1][opt2]{arg1}[opt3]{arg2}[opt4]
```

Therein,

- opt1 is the preferred location of the float, e.g. tbh
- opt2 is the fraction of the linewidth the figure should cover. It can be a value between 0 and 1
- arg1 is the file name of the figure
- opt3 is the short caption for the List of Figures
- arg2 is the caption of the figure in the text
- opt4 is the label of the figure

Abb. 1.7: *This is the caption of the Figure in the text. Is is placed* below *the Figure. It can be longer here and contain additional information, such as references or keys for the graphs. Note that one line captions are justified. A full stop is automatically added after the last sign.*

1.10.3 Tables

A template for a Table is given in Tab. 1.1. Tabelle 1.1 should not be abbreviated at the beginning of a sentence.

Tab. 1.1: *This is the caption of the Table in the text. Is is placed* above *the table. It can be longer and contain additional information. Vertical lines should be avoided in tables. A full stop is automatically added after the last sign.*

Entry 1 Unit 1	Entry 2 Unit 2	Entry 3 Unit 3
1	2	3
4	5	6

1.10.4 References

In the following, a few examples of the authoryear short reference are stated. For more information, the reader is referred to the documentation of the `biblatex` package. Biblatex is used because it is compatible with UTF8. Hence, Umlaute, such as ä, do not have to be rewritten as was the case in bibtex. Example: (Müller, 2018), see .bib file. In addition, biblatex supports editing of the citation style via TEX and LATEX commands. Hence, the tedious editing of bibliography styles (.bst files), which were used with bibtex, is not necessary anymore.

- books: (Coker, 2007, S. 221), Coker (2007, S. 221)
- articles: (Abrams und Prausnitz, 1975), Abrams und Prausnitz (1975)
- conference paper: (Penteado u. a., 2018), Penteado u. a. (2018)
- online: (NIST Chemistry Webbook, 2017), NIST Chemistry Webbook (2017)
- dissertations: (Cuda, 2012), Cuda (2012)
- bachelor/master thesis: (Hoffmann, 2015), Hoffmann (2015)

These commands are used as

- `\textcite{bibtexkey}`: „Abrams und Prausnitz (1975) stated that thermodynamics are great.“
- `\parencite{bibtexkey}`: „Thermodynamics are great (Abrams und Prausnitz, 1975).“

1.10.5 Equations

An exemplary Equation is given in Gl. (1.1). Gleichung (1.1) should not be abbreviated at the beginning of a sentence. The efficient used commands to

generate the partial derivative were made with the `xparse` package.

$$\left(\frac{\partial^2 f}{\partial x^2}\right) = \left[\frac{\partial^4 g}{\partial x^4}\right]. \tag{1.1}$$

For important equations, you might want to use the `empheq` package:

$$\boxed{E = mc^2} \tag{1.2}$$

1.10.6 Theorems, Lemmas, Proofs, Remarks, Definitions, and Algorithms

All of these items are introduced in the following. Note that frames and their colors are arbitrary. You might want to change the color or the linewidth. You can do this in the b_Commands.tex file.

Theorems: Theorems can be defined using the `amsthm` package in combination with the `mdframed` package for a possible frame. An exemplary Theorem is given in Satz 1.1.

Satz 1.1 (What is theoremed): *Let f be a function whose derivative exists in every point, then f is a continuous function.*

Lemmas: Lemmas can be defined using the `amsthm` package in combination with the `mdframed` package for a possible frame. An exemplary Lemma is given in Hilfssatz 1.1.

Hilfssatz 1.1 (What needs to be lemma'd): *Given two line segments whose lengths are a and b, respectively, there is a real number r such that $b = ra$.*

Proofs: Proofs can be defined using the `amsthm` package. They are typically not numerated as they follow a certain Theorem or Lemma.

What needs to be proven. To prove it by contradiction, try and assume that the statement is false, proceed from there, and at some point, you will arrive at a contradiction. □

Remarks: Remarks can be defined using the `amsthm` package in combination with the `mdframed` package for a possible frame. An exemplary Remark is given in Bem. 1.1.

Bemerkung 1.1 (What the remarker remarks): *This statement is true, I guess.*

Definitions: Definitions can be defined using the `amsthm` package in combination with the `mdframed` package for a possible frame. An exemplary Definition is given in Def. 1.1. Gleichung (1.3) can also be referenced.

Definition 1.1 (What the definition defines): *This is a definition. It defines itself.*

$$c = \infty \tag{1.3}$$

Algorithms: Algorithms can be displayed using the algorithm2e package. An example is shown in Alg. 1.1.

Algorithmus 1.1: How to write algorithms

Data: this text
Result: how to write algorithm
initialization;
while *not at end of this document* **do**
    read current;
    if *understand* **then**
        go to next section;
        current section becomes this one;
    else
        go back to the beginning of current section;
    end
end

1.10.7 Autorefs

The `hyperref` package also supplies an `\autoref` command that is linked to babel. In this case, Fig. or Tab. are localized and you do not have to remember whether you used Fig. or Figure or something else in the text. As stated above, at the beginning of a sentence, the long version of an item should be used (the `\Autoref{label}` command was defined for this purpose). Some short forms are equal to their long forms as there is not really a good abbreviation:

a) German ...
   - ..., siehe Kap. 1. Kapitel 1 zeigt, dass ...
   - ..., siehe Abschn. 1.10. Abschnitt 1.10 zeigt, dass ...
   - ..., siehe Abschn. 1.8.1. Abschnitt 1.8.1 zeigt, dass ...
   - ..., siehe Abb. 1.7. Abbildung 1.7 zeigt, dass ...

- ..., siehe Tab. 1.1. Tabelle 1.1 zeigt, dass ...
- ..., siehe Gl. (1.1). Gleichung (1.1) zeigt, dass ...
- ..., siehe Satz 1.1. Satz 1.1 zeigt, dass ...
- ..., siehe Hilfssatz 1.1. Hilfssatz 1.1 zeigt, dass ...
- ..., siehe Bem. 1.1. Bemerkung 1.1 zeigt, dass ...
- ..., siehe Def. 1.1. Definition 1.1 zeigt, dass ...
- ..., siehe Alg. 1.1. Algorithmus 1.1 zeigt, dass ...

b) English ...

- ..., see Chap. 1. Chapter 1 shows that ...
- ..., see Sec. 1.10. Section 1.10 shows that ...
- ..., see Subsec. 1.8.1. Subsection 1.8.1 shows that ...
- ..., see Fig. 1.7. Figure 1.7 shows that ...
- ..., see Tab. 1.1. Table 1.1 shows that ...
- ..., see Eq. (1.1). Equation (1.1) shows that ...
- ..., see Theorem 1.1. Theorem 1.1 shows that ...
- ..., see Lemma 1.1. Lemma 1.1 shows that ...
- ..., see Remark 1.1. Remark 1.1 shows that ...
- ..., see Def. 1.1. Definition 1.1 shows that ...
- ..., see Alg. 1.1. Algorithm 1.1 shows that ...

1.10.8 Acronyms and Abbreviations

New acronyms must typically be explained at their first appearance in the text. The `\ac` command uses the defined acronyms (see List of Abbreviations) for doing that. For example, the **Su**ite of **n**onlinear and **di**fferential-**al**gebraic equation **s**olvers (SUNDIALS) is explained here, but not afterwards because SUNDIALS was already defined. The same is true for a **D**ifferential-**a**lgebraic **e**quation (system) (DAE). Later on, we just write DAE systems. It seems to be more to write, but thus you make sure that an abbreviations is explained

only at its first appearance ... even if you change your text completely. In addition, you link your abbreviations to the List of Abbreviations.

1.10.9 Chemistry and Chemical Reactions

Sometimes it is necessary to state chemical reactions or molecules. For this purpose, the `chemfig` and the `mhchem` package are used as shown in Abb. 1.8.

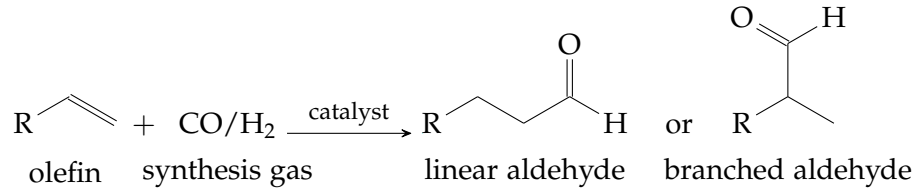


Abb. 1.8: *Hydroformylation reaction scheme to demonstrate the two chemistry packages (based on some reference). Note that the setatomsep command to shorten the bondings was replaced by the author of the chemfig package and should not be used anymore. It is used here to ensure backwards compatibility with older versions of this package.*

1.11 The Sectioning Command for Chapters Supports not only the Heading Text Itself but also a Short Version Whose Use can be Controlled

If your chapters or sections have long titles (which they should not have), you can use an optional argument for chapter or section commands to shorten it in the header. You can even manipulate the chapter or section title. Normally, the use of this option is not necessary.

2 Introduction

Some introducing words ...

2.1 Motivation and Objective

Why this subject is important and what is the goal of this thesis ...

2.2 Literature Review

What are relevant publications in this field and why is their work important for this thesis?

2.3 Outline of Work

What is the structure of this thesis?

3 Theoretical Background

Some introducing words ...

In this chapter, all fundamentals that are necessary to understand this work are introduced.

4 Methods

Dies hier ist ein Blindtext zum Testen von Textausgaben. Wer diesen Text liest, ist selbst schuld. Der Text gibt lediglich den Grauwert der Schrift an. Ist das wirklich so? Ist es gleichgültig, ob ich schreibe: „Dies ist ein Blindtext“ oder „Huardest gefburn“? Kjift – mitnichten! Ein Blindtext bietet mir wichtige Informationen. An ihm messe ich die Lesbarkeit einer Schrift, ihre Anmutung, wie harmonisch die Figuren zueinander stehen und prüfe, wie breit oder schmal sie läuft. Ein Blindtext sollte möglichst viele verschiedene Buchstaben enthalten und in der Originalsprache gesetzt sein. Er muss keinen Sinn ergeben, sollte aber lesbar sein. Fremdsprachige Texte wie „Lorem ipsum“ dienen nicht dem eigentlichen Zweck, da sie eine falsche Anmutung vermitteln. Dies hier ist ein Blindtext zum Testen von Textausgaben. Wer diesen Text liest, ist selbst schuld. Der Text gibt lediglich den Grauwert der Schrift an. Ist das wirklich so? Ist es gleichgültig, ob ich schreibe: „Dies ist ein Blindtext“ oder „Huardest gefburn“? Kjift – mitnichten! Ein Blindtext bietet mir wichtige Informationen. An ihm messe ich die Lesbarkeit einer Schrift, ihre Anmutung, wie harmonisch die Figuren zueinander stehen und prüfe, wie breit oder schmal sie läuft. Ein Blindtext sollte möglichst viele verschiedene Buchstaben enthalten und in der Originalsprache gesetzt sein. Er muss keinen Sinn ergeben, sollte aber lesbar sein. Fremdsprachige Texte wie „Lorem ipsum“ dienen nicht dem eigentlichen Zweck, da sie eine falsche Anmutung vermitteln.

4.1 New Section

Dies hier ist ein Blindtext zum Testen von Textausgaben. Wer diesen Text liest, ist selbst schuld. Der Text gibt lediglich den Grauwert der Schrift an.

Ist das wirklich so? Ist es gleichgültig, ob ich schreibe: „Dies ist ein Blindtext“ oder „Huardest gefburn“? Kjift – mitnichten! Ein Blindtext bietet mir wichtige Informationen. An ihm messe ich die Lesbarkeit einer Schrift, ihre Anmutung, wie harmonisch die Figuren zueinander stehen und prüfe, wie breit oder schmal sie läuft. Ein Blindtext sollte möglichst viele verschiedene Buchstaben enthalten und in der Originalsprache gesetzt sein. Er muss keinen Sinn ergeben, sollte aber lesbar sein. Fremdsprachige Texte wie „Lorem ipsum“ dienen nicht dem eigentlichen Zweck, da sie eine falsche Anmutung vermitteln. Dies hier ist ein Blindtext zum Testen von Textausgaben. Wer diesen Text liest, ist selbst schuld. Der Text gibt lediglich den Grauwert der Schrift an. Ist das wirklich so? Ist es gleichgültig, ob ich schreibe: „Dies ist ein Blindtext“ oder „Huardest gefburn“? Kjift – mitnichten! Ein Blindtext bietet mir wichtige Informationen. An ihm messe ich die Lesbarkeit einer Schrift, ihre Anmutung, wie harmonisch die Figuren zueinander stehen und prüfe, wie breit oder schmal sie läuft. Ein Blindtext sollte möglichst viele verschiedene Buchstaben enthalten und in der Originalsprache gesetzt sein. Er muss keinen Sinn ergeben, sollte aber lesbar sein. Fremdsprachige Texte wie „Lorem ipsum“ dienen nicht dem eigentlichen Zweck, da sie eine falsche Anmutung vermitteln.

4.2 New Section

Dies hier ist ein Blindtext zum Testen von Textausgaben. Wer diesen Text liest, ist selbst schuld. Der Text gibt lediglich den Grauwert der Schrift an. Ist das wirklich so? Ist es gleichgültig, ob ich schreibe: „Dies ist ein Blindtext“ oder „Huardest gefburn“? Kjift – mitnichten! Ein Blindtext bietet mir wichtige Informationen. An ihm messe ich die Lesbarkeit einer Schrift, ihre Anmutung, wie harmonisch die Figuren zueinander stehen und prüfe, wie breit oder schmal sie läuft. Ein Blindtext sollte möglichst viele verschiedene Buchstaben enthalten und in der Originalsprache gesetzt sein. Er muss keinen Sinn ergeben, sollte aber lesbar sein. Fremdsprachige Texte wie „Lorem ipsum“ dienen nicht dem eigentlichen Zweck, da sie eine falsche Anmutung vermitteln. Dies hier ist ein Blindtext zum Testen von Textausgaben. Wer

diesen Text liest, ist selbst schuld. Der Text gibt lediglich den Grauwert der Schrift an. Ist das wirklich so? Ist es gleichgültig, ob ich schreibe: „Dies ist ein Blindtext“ oder „Huardest gefburn“? Kjift – mitnichten! Ein Blindtext bietet mir wichtige Informationen. An ihm messe ich die Lesbarkeit einer Schrift, ihre Anmutung, wie harmonisch die Figuren zueinander stehen und prüfe, wie breit oder schmal sie läuft. Ein Blindtext sollte möglichst viele verschiedene Buchstaben enthalten und in der Originalsprache gesetzt sein. Er muss keinen Sinn ergeben, sollte aber lesbar sein. Fremdsprachige Texte wie „Lorem ipsum“ dienen nicht dem eigentlichen Zweck, da sie eine falsche Anmutung vermitteln.

5 Results and Discussion

6 Conclusion and Outlook

Some introducing words ...

6.1 Conclusion

6.2 Outlook and Future Directions

Literaturverzeichnis

Abrams, D. S. und J. M. Prausnitz (1975). Statistical thermodynamics of liquid mixtures: A new expression for the excess Gibbs energy of partly or completely miscible systems. *AIChE Journal* 21, 116–128. DOI: 10.1002/aic.690210115 (zit. auf S. 20).

Coker, A. K., Hrsg. (2007). *Ludwig's Applied Process Design for Chemical and Petrochemical Plants*. Gulf Professional Publishing. ISBN: 9780080469706 (zit. auf S. 20).

Cuda, P. (2012). Exergoeconomic Analysis and Optimization of Organic Rankine Cycles. *Dissertation*. University of Ontario Institute of Technology. DOI: 10.1016/j.energy.2012.01.064 (zit. auf S. 20).

Hoffmann, C. (2015). Real-time Optimization and Moving-horizon State Estimation for a Hydroformylation Plant. *Masterarbeit*. Technische Universität Berlin (zit. auf S. 20).

Müller, D. (2018). Übertriebene Parameterschätzung. *Chemie Ingenieur Technik* 10, 1–2 (zit. auf S. 20).

NIST Chemistry Webbook (2017). *Benzene - Phase Change Data*. URL: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71432&Units=SI&Mask=4%5C#Thermo-Phase (letzter Zugriff 23. 05. 2016) (zit. auf S. 20).

Penteado, A., H. R. Godini, E. Esche, G. Lovato, J. A. D. Rodrigues und J.-U. Repke (2018). Optimal Design of a CO2 Removal Section for a Biogas-based Oxidative Coupling of Methane Process. In: *Blucher Chemical Engineering Proceedings*. Editora Blucher. DOI: 10.5151/cobeq2018-co.021 (zit. auf S. 20).

A Code Example for AMPL

```
1  reset;  # all blue words are keywords in this language
2          # they are defined in the file 05_Appendix/
               a_CodeLanguageSpecifications.tex
3
4  model simulation.mod;
5  data simulation.dat;
6  include initial.dat;
7  option ipoptoptions "halt_on_ampl_error yes";
8
9  let e0_param := 4;
10
11 solve;
```

Code A.1: *Code example for AMPL.*

B Code Example for Matlab

```
clc
clear
close all

e0_param = 4;

j=0;
for i=1:e0_params % this loop is incredibly smart
    if 1==2
        j=j+1;
    else
        j=j-1;
    end
end
```

Code B.1: *Code example for Matlab.*

C Examples of the longtable Environment

Especially in the appendix, it is common that long tables appear, which contain experimental or simulated data. For this purpose, the `longtable` environment can be used. The `\autoref` command to reference tables works for them as well (Tab. C.1).

Tab. C.1: *This is a longtable, because it is a long table.*

Ragged right Result A	Ragged left Result B	Justified Result C	Parbox Result D
Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.

Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.

Tab. C.2: *The caption of a long table on the first page.*

Ragged right Result A	Ragged left Result B	Justified Result C	Parbox Result D
Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.

Continued on next page

Tab. C.2 (continued).

Ragged right Result A	Ragged left Result B	Justified Result C	Parbox Result D
Text.	Text.	Text.	Longer text to create line breaks.
Text.	Text.	Text.	Longer text to create line breaks.

D Automatic Indenting in arara

In the following, the instructions on using `arara` for automatic indenting are shown for a Windows operating system. It is expected that the instructions are similar on a Unix system, because `arara` is platform independent. Nevertheless, an issue are different versions of `latexindtent` and `arara`. Therefore, instructions are given for version 3.0a of `arara` (TEXLive 2017) and the current version 4.0 (TEXLive 2018). These specific instructions are given in the next two paragraphs. If you have a LATEX distribution from before 2017, we recommend updating LATEX by getting the newest MacTEX, TEXLive, or MiKTEX version.

Arara 3.0a (TEXLive 2017): For TEXLive (and also MikTEX) in this older version, the following steps must be taken to automatically indent the source code:

1. Add a user command for `arara` to Texmaker[1].
2. Add the following command to the beginning of the main.tex file (right before anything else):

```
% arara: indent: { overwrite : yes, files : [ folder/file1.tex,
    folder/file2.tex ] , settings: local, where: 00
   _Arara_and_Latexindent/localSettings.yaml }
```

Code D.1: *Setting up arara for latexindent in Texmaker.*

   This command executes the automatic file indenting for all files (and files in subfolders) that are states within the square brackets. An example is given in Abb. D.1.

[1] https://tex.stackexchange.com/questions/107989/integration-of-arara-in-texmaker, January 2019

3. Add the indent.yaml file that is located in this template folder in 00_Arara_and_Latexindent to your `arara` rules. These rules are typically located in "path_to_texlive/year/texmf-dist/scripts/arara/rules". The .yaml file was taken from a github commit of a `latexindent` developer[2]. He repeatedly pointed out that they do not want to do much backwards compatibility. If you run into issues and this feature is *really important* to you, think about updating your LaTeX distribution (see next paragraph).
4. Execute `arara` (if you added it as the first user command, the shortcut Alt+Shift+F1 may be used).
5. Update your files by clicking on File → Reload all documents from file.
6. Your source code should now be nicely indented.
7. In case errors appear, `arara` always creates a backup with the file extension latexindentbackup.

Arara 4.0 (TeXLive 2018): In 2018, version 4.0 of `arara` was published. With this version, the indent rule is already part of the LaTeX distribution and does not have to be added manually. The procedure is exactly the same as above. You can simply skip step 3 of the instructions. **Problem: Arara 4.0 seems to have an issue with subdirectories. Using it is currently not recommended.**

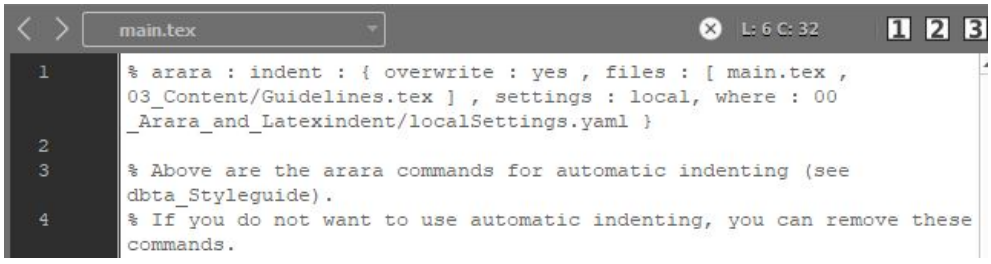


Abb. D.1: *Directives for arara execution for automatic indenting in the main.tex file.*

[2] https://gist.github.com/cereda/3ccdfb6257e5272ad9c1080a89c9ae9b, January 2019

E Package Dependencies

Tab. E.1: *List of all packages in this template.*

Package name	Reference
Document class	
KOMA script	https://ctan.org/pkg/koma-script
Document and encoding	
babel	https://ctan.org/pkg/babel?lang=de
datetime	https://ctan.org/pkg/datetime
fontenc	https://ctan.org/pkg/fontenc
ifthen	https://ctan.org/pkg/ifthen
inputenc	https://ctan.org/pkg/inputenc
microtype	https://ctan.org/pkg/microtype
scrlayer-scrpage	https://ctan.org/pkg/scrlayer-scrpage
xparse	https://ctan.org/pkg/xparse
Tables	
booktabs	https://ctan.org/pkg/booktabs
longtable	https://ctan.org/pkg/longtable
multirow	https://ctan.org/pkg/multirow
tabularx	https://ctan.org/pkg/tabularx
Graphics	
graphicx	https://ctan.org/pkg/graphicx
overpic	https://ctan.org/pkg/overpic
Fonts, math, and symbols	
amsmath	https://ctan.org/pkg/amsmath
amssymb	
amsthm	https://ctan.org/pkg/amsthm

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Tab. E.1 (continued).

cancel	https://ctan.org/pkg/cancel
chemfig	https://ctan.org/pkg/chemfig
courier	https://ctan.org/pkg/courier
empheq	https://ctan.org/pkg/empheq
helvet	https://ctan.org/pkg/helvet?lang=de
icomma	https://ctan.org/pkg/icomma
mathpazo	https://ctan.org/pkg/mathpazo
mathtools	https://ctan.org/pkg/mathtools
mhchem	https://ctan.org/pkg/mhchem
nicefrac	https://ctan.org/pkg/nicefrac
siunitx	https://ctan.org/pkg/siunitx
Text	
algorithm2e	https://ctan.org/pkg/algorithm2e
blindtext	https://ctan.org/pkg/blindtext
caption	https://ctan.org/pkg/caption
enumitem	https://ctan.org/pkg/enumitem
footnote	https://ctan.org/pkg/footnote
mdframed	https://ctan.org/pkg/mdframed
nowidow	https://ctan.org/pkg/nowidow
placeins	https://ctan.org/pkg/placeins
setspace	https://ctan.org/pkg/setspace
subcaption	https://ctan.org/pkg/subcaption
xcolor	https://ctan.org/pkg/xcolor
References	
biblatex	https://ctan.org/pkg/biblatex
csquotes	https://ctan.org/pkg/csquotes
List of Symbols and Abbreviations	
acronym	https://ctan.org/pkg/acronym
nomentbl	https://ctan.org/pkg/nomentbl
Code	
listings	https://ctan.org/pkg/listings
scrhack	

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Tab. E.1 (continued).

Hyperref and pdfx	
hyperref	https://ctan.org/pkg/hyperref
pdfx	https://ctan.org/pkg/pdfx