

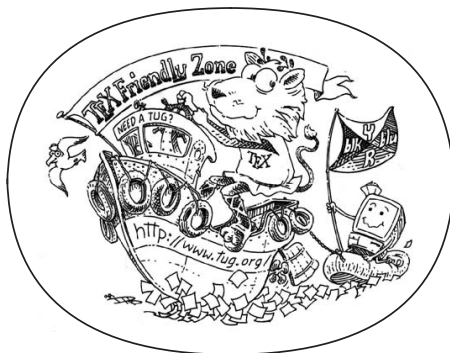
ALI RAMADHAN

MMMGRUBS: MOLECULAR MOTION MOVIES AND  
GEOMETRY RECONSTRUCTION USING BAYESIAN  
STATISTICS



# MMMGRUBS: MOLECULAR MOTION MOVIES AND GEOMETRY RECONSTRUCTION USING BAYESIAN STATISTICS

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An Homage to The Elements of Typographic Style

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## Part I

### HOW TO EXPLODE A MOLECULE

A lot goes into exploding a molecule, even the tiny ones featured here.





## COULOMB EXPLOSION IMAGING

This bundle for L<sup>A</sup>T<sub>E</sub>X has two goals:

1. Provide students with an easy-to-use template for their Master's or PhD thesis. (Though it might also be used by other types of authors for reports, books, etc.)
2. Provide a classic, high-quality typographic style that is inspired by Bringhurst's "*The Elements of Typographic Style*" [2].

The bundle is configured to run with a *full* MiK<sub>T</sub>E<sub>X</sub> or T<sub>E</sub>XLive<sup>1</sup> installation right away and, therefore, it uses only freely available fonts. (Minion fans can easily adjust the style to their needs.)

People interested only in the nice style and not the whole bundle can now use the style stand-alone via the file `classicthesis.sty`. This works now also with "plain" L<sup>A</sup>T<sub>E</sub>X.

As of version 3.0, `classicthesis` can also be easily used with L<sub>Y</sub>X<sup>2</sup> thanks to Nicholas Mariette and Ivo Pletikosić. The L<sub>Y</sub>X version of this manual will contain more information on the details.

This should enable anyone with a basic knowledge of L<sup>A</sup>T<sub>E</sub>X 2<sub>ε</sub> or L<sub>Y</sub>X to produce beautiful documents without too much effort. In the end, this is my overall goal: more beautiful documents, especially theses, as I am tired of seeing so many ugly ones.

The whole template and the used style is released under the GNU General Public License.

If you like the style then I would appreciate a postcard:

André Miede  
Detmolder Straße 32  
31737 Rinteln  
Germany

The postcards I received so far are available at:

<http://postcards.miede.de>

So far, many theses, some books, and several other publications have been typeset successfully with it. If you are interested in some typographic details behind it, enjoy Robert Bringhurst's wonderful book.

MMMGRUBS:  
*Molecular motion  
movies and geometry  
reconstruction using  
Bayesian statistics  
version 4.2*

*A well-balanced line  
width improves the  
legibility of the text.  
That's what  
typography is all  
about, right?*

<sup>1</sup> See the file `LISTOFFILES` for needed packages. Furthermore, `classicthesis` works with most other distributions and, thus, with most systems L<sup>A</sup>T<sub>E</sub>X is available for.

<sup>2</sup> <http://www.lyx.org>

IMPORTANT NOTE: Some things of this style might look unusual at first glance, many people feel so in the beginning. However, all things are intentionally designed to be as they are, especially these:

- No bold fonts are used. Italics or spaced small caps do the job quite well.
- The size of the text body is intentionally shaped like it is. It supports both legibility and allows a reasonable amount of information to be on a page. And, no: the lines are not too short.
- The tables intentionally do not use vertical or double rules. See the documentation for the booktabs package for a nice discussion of this topic.<sup>3</sup>
- And last but not least, to provide the reader with a way easier access to page numbers in the table of contents, the page numbers are right behind the titles. Yes, they are *not* neatly aligned at the right side and they are *not* connected with dots that help the eye to bridge a distance that is not necessary. If you are still not convinced: is your reader interested in the page number or does she want to sum the numbers up?

Therefore, please do not break the beauty of the style by changing these things unless you really know what you are doing! Please.

YET ANOTHER IMPORTANT NOTE: Since classicthesis' first release in 2006, many things have changed in the L<sup>A</sup>T<sub>E</sub>X world. Trying to keep up-to-date, classicthesis grew and evolved into many directions, trying to stay (some kind of) stable and be compatible with its port to L<sub>y</sub>X. However, there are still many remains from older times in the code, many dirty workarounds here and there, and several other things I am absolutely not proud of (for example my unwise combination of KOMA and titlesec etc.).

*An outlook into the  
future of  
classicthesis.*

Currently, I am looking into how to completely re-design and re-implement classicthesis making it easier to maintain and to use. As a general idea, classicthesis.sty should be developed and distributed separately from the template bundle itself. Excellent spin-offs such as arsclassica could also be integrated (with permission by their authors) as format configurations. Also, current trends of microtype, fontspec, etc. should be included as well. As I am not really into deep L<sup>A</sup>T<sub>E</sub>X programming, I will reach out to the L<sup>A</sup>T<sub>E</sub>X community for their expertise and help.

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<sup>3</sup> To be found online at <http://mirror.ctan.org/macros/latex/contrib/booktabs/>.

## 1.1 ORGANIZATION

A very important factor for successful thesis writing is the organization of the material. This template suggests a structure as the following:

*You can use these margins for summaries of the text body...*

- `Chapters/` is where all the “real” content goes in separate files such as `Chapter01.tex` etc.
- `FrontBackMatter/` is where all the stuff goes that surrounds the “real” content, such as the acknowledgments, dedication, etc.
- `gfx/` is where you put all the graphics you use in the thesis. Maybe they should be organized into subfolders depending on the chapter they are used in, if you have a lot of graphics.
- `Bibliography.bib`: the Bib<sub>T</sub>E<sub>X</sub> database to organize all the references you might want to cite.
- `classicthesis.sty`: the style definition to get this awesome look and feel. Does not only work with this thesis template but also on its own (see folder `Examples`). Bonus: works with both L<sub>A</sub>T<sub>E</sub>X and PDF<sub>L</sub>A<sub>T</sub>E<sub>X</sub>...and L<sub>Y</sub>X.
- `ClassicThesis.tcp` a T<sub>E</sub>XnicCenter project file. Great tool and it's free!
- `ClassicThesis.tex`: the main file of your thesis where all gets bundled together.
- `classicthesis-config.tex`: a central place to load all nifty packages that are used.

*Make your changes and adjustments here.* This means that you specify here the options you want to load `classicthesis.sty` with. You also adjust the title of your thesis, your name, and all similar information here. Refer to [Section 1.3](#) for more information.

This had to change as of version 3.0 in order to enable an easy transition from the “basic” style to L<sub>Y</sub>X.

In total, this should get you started in no time.

## 1.2 STYLE OPTIONS

There are a couple of options for `classicthesis.sty` that allow for a bit of freedom concerning the layout:

*...or your supervisor might use the margins for some comments of her own while reading.*

- General:
  - `drafting`: prints the date and time at the bottom of each page, so you always know which version you are dealing with. Might come in handy not to give your Prof. that old draft.
- Parts and Chapters:
  - `parts`: if you use Part divisions for your document, you should choose this option. (Cannot be used together with `nochapters`.)
  - `nochapters`: allows to use the look-and-feel with classes that do not use chapters, e.g., for articles. Automatically turns off a couple of other options: `eulerchapternumbers`, `linedheaders`, `listsseparated`, and `parts`.
  - `linedheaders`: changes the look of the chapter headings a bit by adding a horizontal line above the chapter title. The chapter number will also be moved to the top of the page, above the chapter title.
- Typography:
  - `eulerchapternumbers`: use figures from Hermann Zapf's Euler math font for the chapter numbers. By default, old style figures from the Palatino font are used.
  - `beramono`: loads Bera Mono as typewriter font. (Default setting is using the standard CM typewriter font.)
  - `eulermath`: loads the awesome Euler fonts for math. Palatino is used as default font.
  - `pdfspacing`: makes use of `pdftex`' letter spacing capabilities via the `microtype` package.<sup>4</sup> This fixes some serious issues regarding math formulæ etc. (e.g., "ß") in headers.
  - `minionprospacing`: uses the internal `textssc` command of the MinionPro package for letter spacing. This automatically enables the `minionpro` option, overriding `pdfspacing`.
- Table of Contents:
  - `tocaligned`: aligns the whole table of contents on the left side. Some people like that, some don't.
  - `dottedtoc`: sets `pagenumbers` flushed right in the table of contents.

<sup>4</sup> Use `microtype`'s `DVIoutput` option to generate DVI with `pdftex`.

- `manychapters`: if you need more than nine chapters for your document, you might not be happy with the spacing between the chapter number and the chapter title in the Table of Contents. This option allows for additional space in this context. However, it does not look as “perfect” if you use `\parts` for structuring your document.
- Floats:
  - `listings`: loads the `listings` package (if not already done) and configures the List of Listings accordingly.
  - `floatperchapter`: activates numbering per chapter for all floats such as figures, tables, and listings (if used).
  - `subfig(ure)`: is passed to the `tocloft` package to enable compatibility with the `subfig(ure)` package. Use this option if you want use `classicthesis` with the `subfig` package.

The best way to figure these options out is to try the different possibilities and see what you and your supervisor like best.

In order to make things easier, `classicthesis-config.tex` contains some useful commands that might help you.

### 1.3 CUSTOMIZATION

This section will show you some hints how to adapt `classicthesis` to your needs.

The file `classicthesis.sty` contains the core functionality of the style and in most cases will be left intact, whereas the file `classicthesis-config.tex` is used for some common user customizations.

The first customization you are about to make is to alter the document title, author name, and other thesis details. In order to do this, replace the data in the following lines of `classicthesis-config.tex`:

```
% *****
% 2. Personal data and user ad-hoc commands
% *****
\newcommand{\myTitle}{A Classic Thesis Style\xspace}
\newcommand{\mySubtitle}{An Homage to...\xspace}
```

*Modifications in  
classic-  
thesis-config.tex*

Further customization can be made in `classicthesis-config.tex` by choosing the options to `classicthesis.sty` (see [Section 1.2](#)) in a line that looks like this:

```
\PassOptionsToPackage{eulerchapternumbers,drafting,listings,  
subfig,eulermath,parts}{classicthesis}
```

Many other customizations in `classicthesis-config.tex` are possible, but you should be careful making changes there, since some changes could cause errors.

*Modifications in  
classicthesis.sty*

Finally, changes can be made in the file `classicthesis.sty`, although this is mostly not designed for user customization. The main change that might be made here is the text-block size, for example, to get longer lines of text.

#### 1.4 ISSUES

This section will list some information about problems using `classicthesis` in general or using it with other packages.

Beta versions of `classicthesis` can be found at Bitbucket:

<https://bitbucket.org/amiede/classicthesis/>

There, you can also post serious bugs and problems you encounter.

##### *Compatibility with the glossaries Package*

If you want to use the `glossaries` package, take care of loading it with the following options:

```
\usepackage[style=long,nolist]{glossaries}
```

Thanks to Sven Staehs for this information.

##### *Compatibility with the (Spanish) babel Package*

Spanish languages need an extra option in order to work with this template:

```
\usepackage[spanish,es-lcroman]{babel}
```

Thanks to an unknown person for this information (via the issue reporting).

FURTHER INFORMATION FOR USING `classicthesis` WITH SPANISH (IN ADDITION TO THE ABOVE) In the file `ClassicThesis.tex` activate the language:

```
\selectlanguage{spanish}
```

If there are issues changing `\tablename`, e. g., using this:

```
\renewcommand{\tablename}{Tabla}
```

This can be solved by passing `es-tabla` parameter to `babel`:

```
\PassOptionsToPackage{es-tabla,spanish,es-lcroman,english}{  
  babel}  
\usepackage{babel}
```

But it is also necessary to set `spanish` in the `\documentclass`. Thanks to Alvaro Jaramillo Duque for this information.

### *Compatibility with the pdfsync Package*

Using the pdfsync package leads to linebreaking problems with the graffito command. Thanks to Henrik Schumacher for this information.

## 1.5 FUTURE WORK

So far, this is a quite stable version that served a couple of people well during their thesis time. However, some things are still not as they should be. Proper documentation in the standard format is still missing. In the long run, the style should probably be published separately, with the template bundle being only an application of the style. Alas, there is no time for that at the moment. . . it could be a nice task for a small group of L<sup>A</sup>T<sub>E</sub>Xnicians.

Please do not send me email with questions concerning L<sup>A</sup>T<sub>E</sub>X or the template, as I do not have time for an answer. But if you have comments, suggestions, or improvements for the style or the template in general, do not hesitate to write them on that postcard of yours.

## 1.6 BEYOND A THESIS

The layout of classicthesis.sty can be easily used without the framework of this template. A few examples where it was used to typeset an article, a book or a curriculum vitae can be found in the folder Examples. The examples have been tested with latex and pdflatex and are easy to compile. To encourage you even more, PDFs built from the sources can be found in the same folder.

## 1.7 LICENSE

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