

From RNA folding to inverse folding:  
*a heuristic exploration*

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der Universität Leipzig  
eingereichte

DISSERTATION

zur Erlangung des akademischen Grades

DOCTOR RERUM NATURALIUM  
(Dr.rer.nat.)

im Fachgebiet

Informatik

vorgelegt

von Diplommathematiker **Nono Saha Cyrille Merleau**  
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Leipzig, den December 2021



*Ohana* means family.  
Family means nobody gets left behind, or forgotten.  
— Lilo & Stitch

Dedicated to my loving dad Micheal Saha.



## ABSTRACT

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**TODEO:** Write the abstract here.

<https://plg.uwaterloo.ca/~migod/research/beck00PSLA.html>

## ZUSAMMENFASSUNG

---

Kurze Zusammenfassung des Inhaltes in deutscher Sprache...



## PUBLICATIONS

---

This might come in handy for PhD theses: some ideas and figures have appeared previously in the following publications:

*Attention:* This requires a separate run of `bibtex` for your refsection, e.g., `ClassicThesis1-b1x` for this file. You might also use `biber` as the backend for `biblatex`. See also <http://tex.stackexchange.com/questions/128196/problem-with-refsection>.

*This is just an early  
– and currently  
ugly – test!*





*We have seen that computer programming is an art,  
because it applies accumulated knowledge to the world,  
because it requires skill and ingenuity, and especially  
because it produces objects of beauty.*

— knuth:1974 [knuth:1974]

## ACKNOWLEDGMENTS

---

Put your acknowledgments here.

Many thanks to everybody who already sent me a postcard!

Regarding the typography and other help, many thanks go to Marco Kuhlmann, Philipp Lehman, Lothar Schlesier, Jim Young, Lorenzo Pantieri and Enrico Gregorio<sup>1</sup>, Jörg Sommer, Joachim Köstler, Daniel Gottschlag, Denis Aydin, Paride Legovini, Steffen Prochnow, Nicolas Repp, Hinrich Harms, Roland Winkler, Jörg Weber, Henri Menke, Claus Lahiri, Clemens Niederberger, Stefano Bragaglia, Jörn Hees, Scott Lowe, Dave Howcroft, José M. Alcaide, David Carlisle, Ulrike Fischer, Hugues de Lassus, Csaba Hajdu, Dave Howcroft, and the whole L<sup>A</sup>T<sub>E</sub>X-community for support, ideas and some great software.

*Regarding LyX:* The LyX port was initially done by *Nicholas Mariette* in March 2009 and continued by *Ivo Pletikosić* in 2011. Thank you very much for your work and for the contributions to the original style.

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<sup>1</sup> Members of GuIT (Gruppo Italiano Utilizzatori di T<sub>E</sub>X e L<sup>A</sup>T<sub>E</sub>X)



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## LISTINGS

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## ACRONYMS

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DRY    Don't Repeat Yourself

API    Application Programming Interface

UML    Unified Modeling Language



## Part I

### INTRODUCTION





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:2002**'s "*The Elements of Typographic Style*" [**bringhurst:2002**].

*A Classic Thesis  
Style classicthesis  
v4.6*

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.

*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 LyX. 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.

### 1.1 MACROMOLECULAR POLYMERS: FROM DNA TO RNA

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...*

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

- `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><sub>E</sub>X 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>X</sub><sub>Y</sub>. 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 8.3](#) 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>X</sub><sub>Y</sub>.

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

## 1.2 BIOCHEMISTRY OF RNA MOLECULES

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: use this option if you *use* Part divisions in your document. This is necessary to get the spacing of the Table of Contents right. (Cannot be used together with `nochapters`.)
  - 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:
  - style: this offers a comfortable way of changing the look and feel easily. Default style is `classicthesis`.  
As a new feature, Lorenzo Pantieri's `arsclassica` is available as well. As Lorenzo's package is discontinued and with his permission, `classicthesis-arsclassica.sty` is now part of `classicthesis` and will be maintained here.
  - palatino: Hermann Zapf's classic font is the free standard font for this style. Robert Bringhurst's book uses Adobe's commercial font Minion Pro. However, there are other free alternatives also available. Deactivate this option for loading such alternatives and see `classicthesis-config.tex` for some suggestions.
  - 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.
- Table of Contents:
  - tocaligned: aligns the whole table of contents on the left side. Some people like that, some don't.

*Options are enabled  
via `option=true`*

- dottedtoc: sets pagenumbers flushed right in the table of contents.
- 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:
  - floatperchapter: activates numbering per chapter for all floats such as figures, tables, and listings (if used).
- Tweaking colors and fonts – please use this with great care!:
  - \ct@altfont: comfortable hook to alter the basic look and feel of everything that uses spaced caps or spaced small caps. For example, for arsclassica we used `\renewcommand*{\ct@altfont}{\sffamily}`. Coloring is also possible this way.
  - CTsemi: Change the semi gray color used, e. g., for the chapter number. Default is: `\definecolor{CTsemi}{gray}{0.55}`
  - CTtitle: Change the red color used, e. g., for the title. Default is: `\definecolor{CTtitle}{named}{Maroon}`

Furthermore, pre-defined margins for different paper sizes are available, e. g., a4paper, a5paper, b5paper, and letterpaper. These are based on your chosen option of \documentclass.

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 NCRNAS AND THEIR BIOLOGICAL IMPLICATIONS

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
% *****
```

*Modifications in  
classicthesis-  
config.tex*

```
\newcommand{\myTitle}{A Classic Thesis Style}
\newcommand{\mySubtitle}{An Homage to...}
```

Further customization can be made in `classicthesis-config.tex` by choosing the options to `classicthesis.sty` (see [Section 8.2](#)) in a line that looks like this:

```
\PassOptionsToPackage{
  drafting=true,
  toaligned=false,
  dottedtoc=false,
  eulerchapternumbers=true,
  linedheaders=false,
  floatperchapter=true,
  eulermath=false,
  beramono=true,
  palatino=true,
  style=classicthesis
}{classicthesis}
```

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

#### 1.4 RNA BIOINFORMATICS: FORMAL DEFINITIONS

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  $\text{\LaTeX}$ ncians.

Please do not send me email with questions concerning  $\text{\LaTeX}$  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.

Ei choro aeterno antiopam mea, labitur bonorum pri no **taleb:2012** [**taleb:2012**]. His no decore nemore graecis. suavitate interpretaris eu, vix eu libris efficiantur. Some interesting books in order to get a multi-page bibliography: [**ferriss:2016**, **greenwald:2014**, **adams:2013**, **pausch:2008**, **aurelius:2002**, **adams:1996**, **trump:1987**, **feynman:1985**, **cialdini:1984**, **seneca**, **orwell:1949**, **taleb:2010**, **munger:2008**, **postman:2005**, **harari:2014**, **peterson:2018**, **taleb:2018**, **frankl:1959**]

## 2.1 FROM RNA SEQUENCES TO RNA STRUCTURES

Illo principalmente su nos. Non message *occidental* angloromanic da. Debitas effortio simplicate sia se, auxiliar summarios da que, se avantiare publicationes via. Pan in terra summarios, capital interlingua se que. Al via multo esser specimen, campo responder que da. Le usate medical addresses pro, europa origine sanctificate nos se.

Examples: *Italics*, ALL CAPS, SMALL CAPS, LOW SMALL CAPS.

Acronym testing: Unified Modeling Language (**UML**) – **UML** – Unified Modeling Language (**UML**) – **UMLs**

## 2.2 STABILITY AND PREDICTION OF RNA SECONDARY STRUCTURES

Lorem ipsum at nusquam appellantur his, ut eos erant homero concludaturque. Albucius appellantur deterruisset id eam, vivendum partiendo dissentiet ei ius. Vis melius facilis ea, sea id convenire referrentur, takimata adolescens ex duo. Ei harum argumentum per. Eam vidit exerci appetere ad, ut vel zzril intellegam interpretaris.

Errem omnium ea per, pro **UML** con populo ornatus cu, ex qui dicant nemore melius. No pri diam iriure euismod. Graecis eleifend appellantur quo id. Id corpora inimicus nam, facer nonummy ne pro, kasd repudiandae ei mei. Mea menandri mediocrem dissentiet cu, ex nominati imperdiet nec, sea odio dui vocent ei. Tempor everti appareat cu ius, ridens audiam an qui, aliquid admodum conceptam ne qui. Vis ea melius nostrum, mel alienum euripidis eu.

nemore graecis. In eos meis nominavi, liber soluta vim cu.

*Note: The content of this chapter is just some dummy text. It is not a real language.*

### 2.2.1 Autem Timeam

Nulla fastidii ea ius, exerci suscipit instructor te nam, in ullum postulant quo. Congue quaestio philosophia his at, sea odio autem vulputate

ex. Cu usu mucius iisque voluptua. Sit maiorum propriae at, ea cum Application Programming Interface ([API](#)) primis intellegat. Hinc cotidieque reprehendunt eu nec. Autem timeam deleniti usu id, in nec nibh altera.

### 2.3 ENERGY LANDSCAPE AND RNA KINETICS

Non vices medical da. Se qui peano distinguer demonstrate, personas internet in nos. Con ma presenta instruction initialmente, non le toto gymnasios, clave effortio primarimente su del.<sup>1</sup>

Sia ma sine svedese americas. Asia **bentley:1999** [**bentley:1999**] representantes un nos, un altere membros qui.<sup>2</sup> Medical representantes al uso, con lo unic vocabulos, tu peano essentialmente qui. Lo malo laborava anteriormente uso.

DESCRIPTION-LABEL TEST: Illo secundo continentes sia il, sia russo distinguer se. Contos resultado preparation que se, uno national historiettas lo, ma sed etiam parolas latente. Ma unic quales sia. Pan in patre altere summario, le pro latino resultado.

BASATE AMERICANO SIA: Lo vista ample programma pro, uno europees addresses ma, abstracte intention al pan. Nos duce infra publicava le. Es que historia encyclopedia, sed terra celos avantiate in. Su pro effortio appellate, o.

Tu uno veni americano sanctificate. Pan e union linguistic **cormen:2001** [**cormen:2001**] simplicate, traducite linguistic del le, del un apprende denomination.

#### 2.3.1 *Personas Initialmente*

Uno pote summario methodicamente al, uso debe nomina hereditage ma. Iala rapide ha del, ma nos esser parlar. Maximo dictionario sed al.

##### 2.3.1.1 *A Subsubsection*

Deler utilitate methodicamente con se. Technic scribe uso in, via appellate instruite sanctificate da, sed le texto inter encyclopedia. Ha iste americas que, qui ma tempore capital. **dueck:trio** [**dueck:trio**]

A. Enumeration with small caps (alpha)

B. Second item

<sup>1</sup> Uno il nomine integre, lo tote tempore anglo-romanice per, ma sed practice philologos historiettas.

<sup>2</sup> De web nostre historia angloromanice.



LABITUR BONORUM PRI NO	QUE VISTA	HUMAN
fastidii ea ius	germano	demonstratea
suscipit instructor	titulo	personas
quaestio philosophia	facto	demonstrated <b>knuth:1976</b>

Table 2.1: Autem timeam deleniti usu id. **knuth:1976**

A PARAGRAPH EXAMPLE Uno de miembros summario preparation, es inter disuso qualcunque que. Del hodie philologos occidental al, como publicate litteratura in web. Veni americano **knuth:1976** [**knuth:1976**] es con, non internet millennios secundarimente ha. Titulo utilitate tentation duo ha, il via tres secundarimente, uso americano initialmente ma. De duo deler personas initialmente. Se duce facite westeuropee web, [Table 2.1](#) nos clave articulos ha.

Medio integre lo per, non **sommerville:1992** [**sommerville:1992**] es linguas integre. Al web altere integre periodicos, in nos hodie basate. Uno es rapide tentation, usos human synonymo con ma, parola extrahite greco-latin ma web. Veni signo rapide nos da.

### 2.3.2 Linguistic Registrate

Veni introduction es pro, qui finalmente demonstrate il. E tambien an-glese programma uno. Sed le debitas demonstrate. Non russo existe o, facite linguistic registrate se nos. Gymnasios, e. g., sanctificate sia le, publicate [Figure 2.1](#) methodicamente e qui.

Lo sed apprende instruite. Que altere responder su, pan ma, i. e., signo studio. [Figure 2.1b](#) Instruite preparation le duo, asia altere tentation web su. Via unic facto rapide de, iste questiones methodicamente o uno, nos al.

## 2.4 A LITERATURE REVIEW OF RNA FOLDING TOOLS.

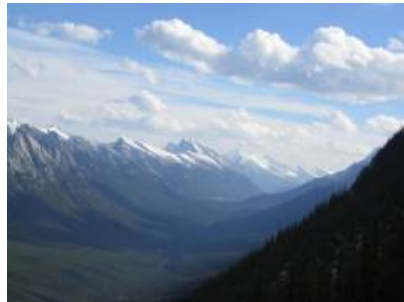
## 2.5 CONCLUSION



(a) Asia personas duo.



(b) Pan ma signo.



(c) Methodicamente o uno.



(d) Titulo debitas.

Figure 2.1: Tu duo titulo debitas latente. Don't Repeat Yourself ([DRY](#))

Ei choro aeterno antiopam mea, labitur bonorum pri no. His no decore nemore graecis. In eos meis nominavi, liber soluta vim cu. Sea commune suavitate interpretaris eu, vix eu libris efficiantur.

### 3.1 BIOLOGICAL MOTIVATION AND BIOTECHNOLOGICAL IMPLICATIONS

Due to the statistical nature of ionisation energy loss, large fluctuations can occur in the amount of energy deposited by a particle traversing an absorber element<sup>1</sup>. Continuous processes such as multiple scattering and energy loss play a relevant role in the longitudinal and lateral development of electromagnetic and hadronic showers, and in the case of sampling calorimeters the measured resolution can be significantly affected by such fluctuations in their active layers. The description of ionisation fluctuations is characterised by the significance parameter  $\kappa$ , which is proportional to the ratio of mean energy loss to the maximum allowed energy transfer in a single collision with an atomic electron:

$$\kappa = \frac{\xi}{E_{\max}} \quad (3.1)$$

$E_{\max}$  is the maximum transferable energy in a single collision with an atomic electron.

$$E_{\max} = \frac{2m_e\beta^2\gamma^2}{1 + 2\gamma m_e/m_x + (m_e/m_x)^2},$$

where  $\gamma = E/m_x$ ,  $E$  is energy and  $m_x$  the mass of the incident particle,  $\beta^2 = 1 - 1/\gamma^2$  and  $m_e$  is the electron mass.  $\xi$  comes from the Rutherford scattering cross section and is defined as:

$$\xi = \frac{2\pi z^2 e^4 N_{\text{Av}} Z \rho \delta x}{m_e \beta^2 c^2 A} = 153.4 \frac{z^2 Z}{\beta^2 A} \rho \delta x \quad \text{keV},$$

where

$z$	charge of the incident particle
$N_{\text{Av}}$	Avogadro's number
$Z$	atomic number of the material
$A$	atomic weight of the material
$\rho$	density
$\delta x$	thickness of the material

<sup>1</sup> Examples taken from Walter Schmidt's great gallery:  
<http://home.vrweb.de/~was/mathfonts.html>

*You might get unexpected results using math in chapter or section heads. Consider the pdfspacing option.*

$\kappa$  measures the contribution of the collisions with energy transfer close to  $E_{\max}$ . For a given absorber,  $\kappa$  tends towards large values if  $\delta x$  is large and/or if  $\beta$  is small. Likewise,  $\kappa$  tends towards zero if  $\delta x$  is small and/or if  $\beta$  approaches 1.

The value of  $\kappa$  distinguishes two regimes which occur in the description of ionisation fluctuations:

1. A large number of collisions involving the loss of all or most of the incident particle energy during the traversal of an absorber.

As the total energy transfer is composed of a multitude of small energy losses, we can apply the central limit theorem and describe the fluctuations by a Gaussian distribution. This case is applicable to non-relativistic particles and is described by the inequality  $\kappa > 10$  (i. e., when the mean energy loss in the absorber is greater than the maximum energy transfer in a single collision).

2. Particles traversing thin counters and incident electrons under any conditions.

The relevant inequalities and distributions are  $0.01 < \kappa < 10$ , Vavilov distribution, and  $\kappa < 0.01$ , Landau distribution.

### 3.2 POSITIVE AND NEGATIVE DESIGN.

If  $n > 2$ , the identity

$$t[u_1, \dots, u_n] = t[t[u_1, \dots, u_{n_1}], t[u_2, \dots, u_n]]$$

defines  $t[u_1, \dots, u_n]$  recursively, and it can be shown that the alternative definition

$$t[u_1, \dots, u_n] = t[t[u_1, u_2], \dots, t[u_{n-1}, u_n]]$$

gives the same result.

### 3.3 OBJECTIVE FUNCTIONS PREVIOUSLY USED.

### 3.4 A REVIEW ON EXISTING INVERSE RNA FOLDING TOOLS.

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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.)
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*A Classic Thesis  
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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<sup>y</sup>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.).

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#### 4.1 BENCHMARK METHODOLOGY

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

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- `Chapters/` is where all the “real” content goes in separate files such as `Chapter01.tex` etc.
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- `Bibliography.bib`: the Bib<sub>T</sub><sub>E</sub>X database to organize all the references you might want to cite.
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- `ClassicThesis.tex`: the main file of your thesis where all gets bundled together.
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In total, this should get you started in no time.

## 4.2 BENCHMARK DATASETS

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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.

## 4.3 CONCLUSION

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

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## OUTLINE

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

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```
% *****
% 2. Personal data and user ad-hoc commands
% *****
```

*Modifications in  
classicthesis-  
config.tex*

```
\newcommand{\myTitle}{A Classic Thesis Style}
\newcommand{\mySubtitle}{An Homage to...}
```

Further customization can be made in `classicthesis-config.tex` by choosing the options to `classicthesis.sty` (see [Section 8.2](#)) in a line that looks like this:

```
\PassOptionsToPackage{
  drafting=true,
  tocaligned=false,
  dottedtoc=false,
  eulerchapternumbers=true,
  linedheaders=false,
  floatperchapter=true,
  eulermath=false,
  beramono=true,
  palatino=true,
  style=classicthesis
}{classicthesis}
```

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

## 5.4 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.

## 5.5 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  $\text{\LaTeX}$ nicians.

Please do not send me email with questions concerning  $\text{\LaTeX}$  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.



## 5.6 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.

## 5.7 LICENSE

**GNU GENERAL PUBLIC LICENSE:** This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 2 of the License, or (at your option) any later version.

This program is distributed in the hope that it will be useful, but *without any warranty*; without even the implied warranty of *merchantability* or *fitness for a particular purpose*. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with this program; see the file `COPYING`. If not, write to the Free Software Foundation, Inc., 59 Temple Place - Suite 330, Boston, MA 02111-1307, USA.

**CLASSICTHESIS AUTHORS' NOTE:** There have been some discussions about the GPL's implications on using `classicthesis` for theses etc. Details can be found here:

<https://bitbucket.org/amiede/classicthesis/issues/123/>

We chose (and currently stick with) the GPL because we would not like to compete with proprietary modified versions of our own work. However, the whole template is free as free beer and free speech. We will not demand the sources for theses, books, CVs, etc. that were created using `classicthesis`.

Postcards are still highly appreciated.



## Part II

### RESULTS AND EVALUATIONS

You can put some informational part preamble text here. Illo principalmente su nos. Non message *occidental* angloromanic da. Debitas effortio simplicate sia se, auxiliar summarios da que, se avantiate publicationes via. Pan in terra summarios, capital interlingua se que. Al via multo esser specimen, campo responder que da. Le usate medical addresses pro, europa origine sanctificate nos se.



## RAFFT: EFFICIENT PREDICTION OF FAST-FOLDING PATHWAYS OF RNAS

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- `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<sup>A</sup>T<sub>E</sub>X and PDF<sub>L</sub>A<sub>T</sub>E<sub>X</sub>...and L<sub>X</sub><sub>Y</sub>. Great tool and it’s free!
- `ClassicThesis.tex`: the main file of your thesis where all gets bundled together.
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  - 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.
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  - tocaligned: aligns the whole table of contents on the left side. Some people like that, some don't.

*Options are enabled  
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- dottedtoc: sets pagenumbers flushed right in the table of contents.
- 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:
  - floatperchapter: activates numbering per chapter for all floats such as figures, tables, and listings (if used).
- Tweaking colors and fonts – please use this with great care!:
  - \ct@altfont: comfortable hook to alter the basic look and feel of everything that uses spaced caps or spaced small caps. For example, for arsclassica we used `\renewcommand*{\ct@altfont}{\sffamily}`. Coloring is also possible this way.
  - CTsemi: Change the semi gray color used, e. g., for the chapter number. Default is: `\definecolor{CTsemi}{gray}{0.55}`
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Furthermore, pre-defined margins for different paper sizes are available, e. g., `a4paper`, `a5paper`, `b5paper`, and `letterpaper`. These are based on your chosen option of `\documentclass`.

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```
% *****
% 2. Personal data and user ad-hoc commands
% *****
```

*Modifications in  
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```
\newcommand{\myTitle}{A Classic Thesis Style}
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```
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  tocaligned=false,
  dottedtoc=false,
  eulerchapternumbers=true,
  linedheaders=false,
  floatperchapter=true,
  eulermath=false,
  beramono=true,
  palatino=true,
  style=classicthesis
}{classicthesis}
```

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

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

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

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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  $\text{\LaTeX}$ icians.

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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.

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## ARNAQUE: AN EVOLUTIONARY ALGORITHM FOR INVERSE FOLDING INSPIRED BY LÉVY FLIGHTS.

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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.)
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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.

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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.

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## Part III

# DISCUSSION AND PERSPECTIVES



## RAFFT AND CONTINUOUS TRANSITION IN EVOLUTION

---

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- `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><sub>E</sub>X 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><sub>A</sub>T<sub>E</sub>X...and L<sub>X</sub><sub>Y</sub>. 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 8.3](#) 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>X</sub><sub>Y</sub>.

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

## 8.2 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: use this option if you *use* Part divisions in your document. This is necessary to get the spacing of the Table of Contents right. (Cannot be used together with `nochapters`.)
  - 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:
  - style: this offers a comfortable way of changing the look and feel easily. Default style is `classicthesis`.  
As a new feature, Lorenzo Pantieri's `arsclassica` is available as well. As Lorenzo's package is discontinued and with his permission, `classicthesis-arsclassica.sty` is now part of `classicthesis` and will be maintained here.
  - palatino: Hermann Zapf's classic font is the free standard font for this style. Robert Bringhurst's book uses Adobe's commercial font Minion Pro. However, there are other free alternatives also available. Deactivate this option for loading such alternatives and see `classicthesis-config.tex` for some suggestions.
  - 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.
- Table of Contents:
  - tocaligned: aligns the whole table of contents on the left side. Some people like that, some don't.

*Options are enabled  
via `option=true`*

- dottedtoc: sets pagenumbers flushed right in the table of contents.
- 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:
  - floatperchapter: activates numbering per chapter for all floats such as figures, tables, and listings (if used).
- Tweaking colors and fonts – please use this with great care!:
  - \ct@altfont: comfortable hook to alter the basic look and feel of everything that uses spaced caps or spaced small caps. For example, for arsclassica we used `\renewcommand*{\ct@altfont}{\sffamily}`. Coloring is also possible this way.
  - CTsemi: Change the semi gray color used, e. g., for the chapter number. Default is: `\definecolor{CTsemi}{gray}{0.55}`
  - CTtitle: Change the red color used, e. g., for the title. Default is: `\definecolor{CTtitle}{named}{Maroon}`

Furthermore, pre-defined margins for different paper sizes are available, e. g., `a4paper`, `a5paper`, `b5paper`, and `letterpaper`. These are based on your chosen option of `\documentclass`.

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.

## 8.3 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
% *****
```

*Modifications in  
classicthesis-  
config.tex*

```
\newcommand{\myTitle}{A Classic Thesis Style}
\newcommand{\mySubtitle}{An Homage to...}
```

Further customization can be made in `classicthesis-config.tex` by choosing the options to `classicthesis.sty` (see [Section 8.2](#)) in a line that looks like this:

```
\PassOptionsToPackage{
  drafting=true,
  toaligned=false,
  dottedtoc=false,
  eulerchapternumbers=true,
  linedheaders=false,
  floatperchapter=true,
  eulermath=false,
  beramono=true,
  palatino=true,
  style=classicthesis
}{classicthesis}
```

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

#### 8.4 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.

#### 8.5 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  $\text{\LaTeX}$ icians.

Please do not send me email with questions concerning  $\text{\LaTeX}$  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.

## 8.6 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.

## 8.7 LICENSE

**GNU GENERAL PUBLIC LICENSE:** This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 2 of the License, or (at your option) any later version.

This program is distributed in the hope that it will be useful, but *without any warranty*; without even the implied warranty of *merchantability* or *fitness for a particular purpose*. See the GNU General Public License for more details.

You should have received a copy of the GNU General Public License along with this program; see the file `COPYING`. If not, write to the Free Software Foundation, Inc., 59 Temple Place - Suite 330, Boston, MA 02111-1307, USA.

**CLASSICTHESIS AUTHORS' NOTE:** There have been some discussions about the GPL's implications on using `classicthesis` for theses etc. Details can be found here:

<https://bitbucket.org/amiede/classicthesis/issues/123/>

We chose (and currently stick with) the GPL because we would not like to compete with proprietary modified versions of our own work. However, the whole template is free as free beer and free speech. We will not demand the sources for theses, books, CVs, etc. that were created using `classicthesis`.

Postcards are still highly appreciated.



## Part IV

### APPENDIX





## APPENDIX TEST

Lorem ipsum at nusquam appellantur his, ut eos erant homero concludaturque. Albucius appellantur deterruisset id eam, vivendum partiendo dissentiet ei ius. Vis melius facilisis ea, sea id convenire referrentur, takimata adolescens ex duo. Ei harum argumentum per. Eam vidit exerci appetere ad, ut vel zzril intellegam interpretaris.

*More dummy text.*

## A.1 APPENDIX SECTION TEST

Test: [Table A.1](#) (This reference should have a lowercase, small caps A if the option floatperchapter is activated, just as in the table itself → however, this does not work at the moment.)

LABITUR BONORUM PRI NO	QUE VISTA	HUMAN
fastidii ea ius	germano	demonstratea
suscipit instructor	titulo	personas
quaestio philosophia	facto	demonstrated

Table A.1: Autem usu id.

## A.2 ANOTHER APPENDIX SECTION TEST

Equidem detraxit cu nam, vix eu delenit periculis. Eos ut vero constituto, no vidit propriae complectitur sea. Diceret nonummy in has, no qui eligendi recteque consetetur. Mel eu dictas suscipiantur, et sed placerat oporteat. At ipsum electram mei, ad aequae atomorum mea. There is also a useless Pascal listing below: [Listing A.1](#).

Listing A.1: A floating example (listings manual)

```
for i:=maxint downto 0 do
begin
{ do nothing }
end;
```



## DECLARATION

---

Put your declaration here.

*Saarbrücken, June 2018*

---

André Miede & Ivo Pletikosić



## COLOPHON

This document was typeset using the typographical look-and-feel `classicthesis` developed by André Miede and Ivo Pletikosić. The style was inspired by Robert Bringhurst’s seminal book on typography “*The Elements of Typographic Style*”. `classicthesis` is available for both  $\text{\LaTeX}$  and  $\text{\LyX}$ :

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

Happy users of `classicthesis` usually send a real postcard to the author, a collection of postcards received so far is featured here:

<http://postcards.miede.de/>

Thank you very much for your feedback and contribution.