



**GONÇALO GARCÊS SOBREIRA RODRIGUES BAPTISTA**  
BSc in Physics Engineering

## X-RAY RESONANT RAMAN SCATTERING

SPECTRA SIMULATION FROM FIRST PRINCIPLES  
FOR COPPER BELOW IONIZATION THRESHOLD  
USING HIGH-PERFORMANCE COMPUTING

MASTER IN PHYSICS ENGINEERING  
NOVA University Lisbon  
*Draft: December 5, 2022*



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BSc in Physics Engineering

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MASTER IN PHYSICS ENGINEERING

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# Abstract

Throughout this thesis, we will explore the influence that consequently higher excited states will have on Copper's diagram transition lines and their fluorescence yield. Multiple atomic structure calculations will be performed for different excited states configurations (from an electron in the 4s orbital up to n=??). This way, it will be possible to observe the energy shifts and shape changes of Copper's K and L diagram transition lines as they get closer to the ones from ionized Copper. For this purpose, a high performance computational method, [Multiconfiguration Dirac-Fock General Matrix of Elements \(MCD-FGME\)](#), will be used in order to performance the necessary atomic structure calculations and to compute all the transition line's parameters, while also evaluating all the K and L fluorescence yields.

This study can be of high importance since the theoretical results obtained shall be used in order to fully comprehend and analyze experimental data obtained from a high precision [Double Crystal Spectrometer \(DCS\)](#), located in Paris, in a synchroton line.

Further similar and more complex studies will be performed by implementing and running a script in the *Oblivion* supercomputer located at the University of Évora.

**Keywords:** Excited State, Diagram Lines, Fluorescence Yield, [MCDFGME](#), [DCS](#), High Performance Computing

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# Resumo

Independentemente da língua em que a dissertação está escrita, geralmente esta contém pelo menos dois resumos: um resumo na mesma língua do texto principal e outro resumo numa outra língua.

A ordem dos resumos varia de acordo com a escola. O comportamento padrão para o template **NOVAthesis LaTeX** (**novathesis**) é ter em primeiro lugar o resumo *na mesma língua do texto principal* e depois o resumo *na outra língua*. Por exemplo, se a dissertação for escrita em português, a ordem dos resumos será primeiro em português e depois em inglês, seguido do texto principal em português. Se a dissertação for escrita em inglês, a ordem dos resumos será primeiro em inglês e depois em português, seguido do texto principal em inglês. O template **novathesis** (L<sup>A</sup>T<sub>E</sub>X) irá ordenar automaticamente os resumos por uma ordem apropriada. No entanto, esta ordem pode ser personalizada adicionando

```
\abstractorder(<MAIN_LANG>) := {<LANG_1>, ..., <LANG_N>}
```

ao ficheiro `5_packages.tex`. Por exemplo, para um documento escrito em Alemão com resumos em Alemão, Inglês e Italiano (por esta ordem), pode usar-se:

```
\abstractorder(de) := {de, en, it}
```

Relativamente ao seu conteúdo, os resumos não devem ultrapassar uma página e frequentemente tentam responder às seguintes questões (é imprescindível a adaptação às práticas habituais da sua área científica):

1. Qual é o problema?
2. Porque é que é um problema interessante/desafiante?
3. Qual é a proposta de abordagem/solução?
4. Quais são as consequências/resultados da solução proposta?

**Palavras-chave:** Primeira palavra-chave, Outra palavra-chave, Mais uma palavra-chave, A última palavra-chave

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## Glossary

**computer** An electronic device which is capable of receiving information (data) in a particular form and of performing a sequence of operations in accordance with a predetermined but variable set of procedural instructions (program) to produce a result in the form of information or signals. This is a test that adds a citation [2] to the glossary! (*p. 18*)

---

# Acronyms

$\mu$	Mu (p. 18)
<b>MCDFGME</b>	Multiconfiguration Dirac-Fock General Matrix of Elements (p. ii)
<b>aaa</b>	acronym aaa (p. 17)
<b>aab</b>	acronym aab (p. 17)
<b>aba</b>	acronym aba (p. 17)
<b>abbrev</b>	abbreviation of a longer text (p. 17)
<b>bbb</b>	acronym bbb (p. 17)
<b>DCS</b>	Double Crystal Spectrometer (p. ii)
<b>DI</b>	Department of Computer Science (p. 2)
<b>FCT</b>	NOVA School of Science and Technology (pp. 2, 10)
<b>NOVA</b>	NOVA University Lisbon (p. 2)
<b>novathesis</b>	NOVATHESIS LaTeX (pp. iii, vi, vii, 1–4, 6–13)
<b>novathesis.cls</b>	novathesis.cls class (p. 13)
<b>xpto</b>	and extension of a xpto xpto xpto xpto xpto xpto xpto xpto xpto xpto xpto xpto xpto xpto xpto xpto xpto (p. 17)

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## Symbols

$\pi$  the numerical value of pi (*p. 17*)

$r$  the radius of a circle (*p. 17*)

---

## Chemical Symbols

$K^+$  Ião positivo de Potássio (p. 18)

$Na^+$  Ião positivo de Sódio (p. 18)

# Introduction



This is the **novathesis** L<sup>A</sup>T<sub>E</sub>X template Version 6.10.12 from 2022-10-25.

*This work is licensed under the L<sup>A</sup>T<sub>E</sub>X Project Public License v1.3c. To view a copy of this license, visit the [LaTeX project public license](#).*

## 1.1 Welcome to the novathesis Template

This first Chapter introduces the **novathesis** template and how it is organized. In Chapter 2 you can find some specific instructions on how to use the **novathesis** template. Chapter 3 shows some examples and give some hints on how to write your text. Please read these next Chapters carefully.

### 1.1.1 Your Time is Precious

Did you learn how to drive by sitting by the wheel and throwing your car into the road? Most probably you did take your time *learning the rules* and *practicing* first! Likewise, it is not wise to throw yourself at the task of writing a thesis/dissertation in L<sup>A</sup>T<sub>E</sub>X without seriously considering the following statement!

---

*If you are going to spend zillions of hours writing your thesis/dissertation using this novathesis template, be wise and spend a couple of hours learning how to use it properly by reading this manual. And then, be even wiser, and spend a few more hours learning some L<sup>A</sup>T<sub>E</sub>X. I am sure that the time you are investing now will pay itself countless times before you submit your thesis/dissertation.*

---

*João Lourenço*

### 1.1.2 Recognition

The **novathesis** template was born in 1996, and what you see now accumulates to many many hundreds (thousands?!?) of working hours, unpaid and stollen from family and friends. This work is available to the community under the [LaTeX Project Public License v1.3c](#), which means you are entitled to use it for free. However, if you decide to use this template to write your thesis/dissertation, **be fair to the developers** and:

1. Cite the **novathesis** manual [10] in a place of your choice (e.g., in the *Acknowledgments*) of your thesis/dissertation with “`\cite{novathesis-manual}`”. If you cite it this way, the correct entry will be added automatically to your bibliography (no need to worry with the necessary BibTeX entry, as it will be added automatically);
2. Go to the [project web page in GitHub](#) and give the project a star (marked with a red ellipse at the top-right in Figure 1.1); and
3. Make a donation by visiting the **novathesis** project page and clicking in the button marked with a green ellipse at the top-center in Figure 1.1). Alternatively, just click [HERE](#) and your browser will be directed to the right page.

## 1.2 The NOVAthesis template

The **novathesis** template was born at the [Department of Computer Science \(DI\)](#) of [NOVA School of Science and Technology \(FCT\)](#) of [NOVA University Lisbon \(NOVA\)](#), Portugal. But the user base grew... initially to other Departments of FCT-NOVA, then to other Schools of NOVA, and later to other Schools of other Universities. Currently more than 25 Schools are natively supported by the **novathesis** template (see Tables 1.1, 1.2, 1.3, 1.4, 1.5, and 1.6).

Table 1.1: NOVA University Lisbon’s Schools supported by the **novathesis** template

---

NOVA University Lisbon
------------------------



### NOVA School of Science and Technology (FCT-NOVA)

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### NOVA School of Social Sciences and Humanities (FCSH-NOVA)

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### NOVA Information Management School (NOVA-IMS)

- All PhD Programs ([PhD](#))
- Master's in Data Science and Advanced Analytics ([MMAA](#))
- Master's in Statistics and Information Management ([MEGI](#))
- Master's in Information Management ([MGI](#))
- Master's in Geographic Information Systems and Science ([MCSIG](#))
- Master's in Geospatial Technologies ([GeoTech](#))



### National School of Public Health (ENSP-NOVA)

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### Instituto de Tecnologia Química e Biológica (ITQB-NOVA)

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))

Table 1.2: University of Lisbon's Schools supported by the **novathesis** template

University of Lisbon

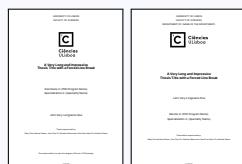
## CHAPTER 1. INTRODUCTION

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### Instituto Superior Técnico (IST-UL)

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### Faculdade de Ciências (FCUL)

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### Faculdade de Medicina Veterinária (FMV-UL)

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))

Table 1.3: University of Minho's Schools supported by the `novatheresis` template

University of Minho
Two sample thesis covers for School of Architecture (EA-UMINHO). The left cover is dark grey with a white header and footer. The right cover is white with a dark grey header and footer. Both covers feature the EA-UMINHO logo and the text 'Escola de Arquitetura' and 'Tese de Mestrado'.
<h3>School of Architecture (EA-UMINHO)</h3> <ul style="list-style-type: none"><li>• All PhD Programs (<a href="#">PhD</a>)</li><li>• All MSc Programs (<a href="#">MSc</a>)</li></ul>
Two sample thesis covers for School of Sciences (EC-UMINHO). The left cover is dark grey with a white header and footer. The right cover is white with a dark grey header and footer. Both covers feature the EC-UMINHO logo and the text 'Escola de Ciências' and 'Tese de Mestrado'.
<h3>School of Sciences (EC-UMINHO)</h3> <ul style="list-style-type: none"><li>• All PhD Programs (<a href="#">PhD</a>)</li><li>• All MSc Programs (<a href="#">MSc</a>)</li></ul>
Two sample thesis covers for School of Law (ED-UMINHO). The left cover is dark grey with a white header and footer. The right cover is white with a dark grey header and footer. Both covers feature the ED-UMINHO logo and the text 'Escola de Direito' and 'Tese de Mestrado'.
<h3>School of Law (ED-UMINHO)</h3> <ul style="list-style-type: none"><li>• All PhD Programs (<a href="#">PhD</a>)</li><li>• All MSc Programs (<a href="#">MSc</a>)</li></ul>
Two sample thesis covers for School of Engineering (EE-UMINHO). The left cover is dark grey with a white header and footer. The right cover is white with a dark grey header and footer. Both covers feature the EE-UMINHO logo and the text 'Escola de Engenharia' and 'Tese de Mestrado'.
<h3>School of Engineering (EE-UMINHO)</h3> <ul style="list-style-type: none"><li>• All PhD Programs (<a href="#">PhD</a>)</li><li>• All MSc Programs (<a href="#">MSc</a>)</li></ul>



### School of Economics and Management ([EEG-UMINHO](#))

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### School of Medicine ([EM-UMINHO](#))

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### School of Psychology ([EP-UMINHO](#))

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### School of Nursing ([ESE-UMINHO](#))

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### Institute of Social Sciences ([ICS-UMINHO](#))

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### Institute of Education ([IE-UMINHO](#))

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### School of Arts and Humanities ([ILCH-UMINHO](#))

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))



### Research Institute 13Bs ([I3B-UMINHO](#))

- All PhD Programs ([PhD](#))
- All MSc Programs ([MSc](#))

## CHAPTER 1. INTRODUCTION

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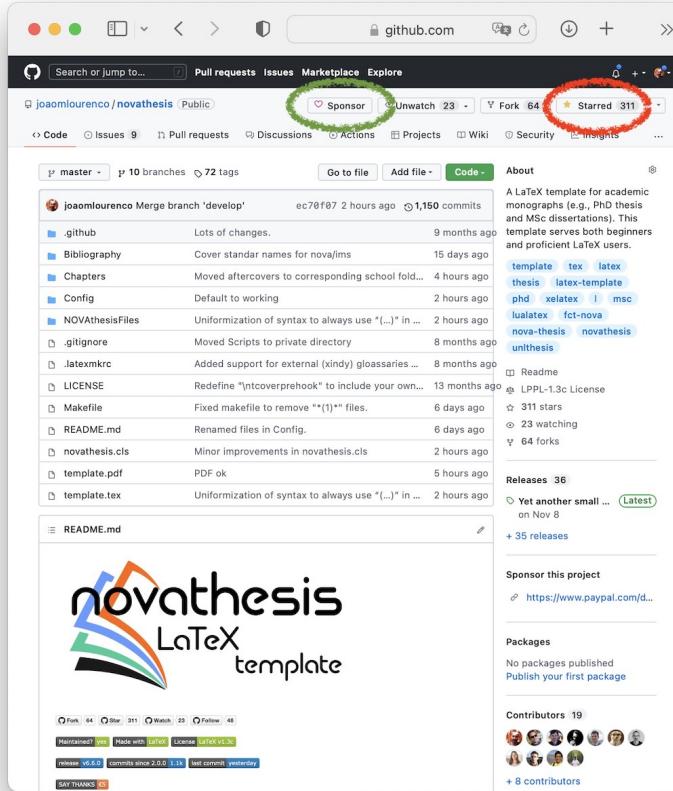


Figure 1.1: The **novathesis** project web page in GitHub.

Table 1.4: Instituto Politécnico de Lisboa's Schools supported by the **novathesis** template

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Instituto Politécnico de Lisboa
---------------------------------



### Instituto Superior de Engenharia de Lisboa (ISEL-IPL)

- All MSc Programs ([MSc](#))

Table 1.5: Instituto Politécnico de Setúbal's Schools supported by the **novathesis** template

---

Instituto Politécnico de Setúbal
----------------------------------



### Escola Superior de Tecnologia de Setúbal (ISEL-IPL)

- All MSc Programs ([MSc](#))

Table 1.6: Other Universities/Schools/Degrees's Schools supported by the **novathesis** template

Other Universities/Schools/Degrees
------------------------------------



### Escola Superior de Enfermagem do Porto (ESEP)

- All MSc Programs ([MSc](#))

## 1.3 Getting Started

The template provides an *easy to use* setting for you to write your thesis/dissertation in **LATEX**:

- Select your school;
- Fill your thesis metadata (title, research field, etc) in the file “`template.tex`”;
- Create your thesis/dissertation contents using the files in folder “Chapters”; and
- Process using you favorite LATEX processor (pdfLATEX, XeLATEX or LuaLATEX).

### 1.3.1 Using Overleaf

If you do not have an account in **Overleaf**, you must [create one first](#).

Once you have an account, please access the **novathesis** template in **Overleaf** and select the green button *Open as Template* (see [Figure 1.2](#)).

*Please notice that the version currently available in Overleaf (v6.5.3) is slightly outdated (current version is v6.10.12). A new version will be submitted to Overleaf soon. Until then, please:*

1. Download the [latest version](#) from the GitHub repository as a Zip file.

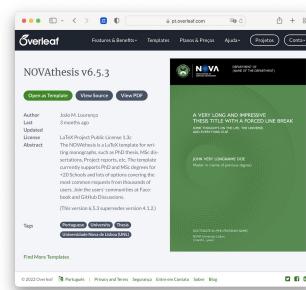


Figure 1.2: NOVAtesis template in Overleaf.

2. Login to your favorite *LaTeX* cloud service. I recommend [Overleaf](#) but there are alternatives (these instructions apply to Overleaf and you'll have to adapt for other providers).
3. In the menu select: *New project* → *Upload project*.
4. Upload the zip file.
5. Select “*template.tex*” as the main file.
6. Let Overleaf compile the document.

### 1.3.2 Using a Local *LATEX* Installation

First of all, start by installing *LATEX* in your computer. There are two main distributions, [MikTeX](#) and [TeXLive](#), and both of them are available for the 3 most popular Operating Systems: Linux, macOS and Windows.

Be aware that a full installation of MikTeX or TeXLive will take near 5 GB of hard disk space. So, think twice before installing the full distribution. See the [novathesis](#) Wiki for the [list of packages required to compile the template](#).

Once you have *LATEX* up and running, remember to install a good *LATEX* text editor. I recommend you to take a look at [this post](#) in the [tex.stackexchange.com](#) site. If you want a quick and dirty recommendation, try [TeXStudio](#).

Now, you must access the [novathesis](#) repository in [GitHub](#), select the green button *Code* and then *download* (or *clone*) the template. You will always get the latest version of the template (currently v6.10.12 from 2022-10-25).

## 1.4 Getting Help

No! You don't have to use this template to write your thesis. You don't even have to use *LATEX*. However, writing a thesis is serious stuff, and which tool you shall use to write it is not a decision to make lighthearted.

*LATEX* is hard enough by itself. This template aims at making your life easier, but not easy. If you choose to use this template to write your thesis, you are very welcome. However, don't expect me to provide you help with *LATEX*. Look for help with your friends (you have some friends, don't you?), or search the web, or try even to read some book(s) on *LATEX*. In the end you will certainly find the experience rewarding.

When you come to the point of “*How do I do this with LATEX?*”, remember...

1. To check the [novathesis](#) [wiki](#) and have some hope! :D
2. Google is your best friend.

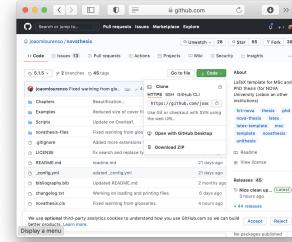


Figure 1.3: The NOVAtesis Project page in GitHub.

3. Search the [GitHub Discussions page](#) for a question related to yours. *If and only if* you don't find one, then post your own question in English please!
4. Search the [NOVAtheis Facebook group](#) for a question related to yours. *If and only if* you don't find one, then post your own question in either Portuguese or English, at your preference.

When you post your own question, remember to **always** state the `novathesis` version number you are using and referring to.

**Please do not attempt to contact me directly (email, Messenger, etc)...**  
**I WILL NOT REPLY!**

#### 1.4.1 Suggestions, Bugs and Feature Requests

**Help:** If you just need some help, see above [Section 1.4](#).

**Suggestion:** Do you have a suggestion/recommendation? Please add it to the wiki and help other users!

**Bug:** Did you find a bug? Please open an issue. Thanks!

**New Feature:** Would you like to request a new feature (or support of a new School)? Please open an issue. Thanks!

### 1.5 Donors

The [list of Donors](#) is available in the `novathesis` Project page.

### 1.6 Disclaimer

Although the `novathesis` template is endorsed by some Schools (e.g., [linked from FCT-NOVA web site](#)), the `novathesis` template **this not an official template** for any School.

The `novathesis` template exists to make your life easier and we do our best to make it compliant to the supported (+25) Schools' regulations but, in the end of the line, you and only you are accountable for both the look and the contents of the document you submit as your thesis/dissertation.

---

# NOVAthesis Template User's Manual

This manual is outdated and must be revised!

## 2.1 Introduction

This Chapter describes how to use the NOVAthesis LaTeX (`novathesis`) template. It is assumed that you have a working installation of L<sup>A</sup>T<sub>E</sub>X, either local (in your own computer) or remote (in Overleaf), and that you were able to generate a PDF for the default configuration of the template: a PhD thesis for NOVA School of Science and Technology (FCT).

## 2.2 Quick Start

### 2.2.1 With a Local L<sup>A</sup>T<sub>E</sub>X Installation

Follow these steps to get started with a local L<sup>A</sup>T<sub>E</sub>X installation:

1. Download L<sup>A</sup>T<sub>E</sub>X. There are two major L<sup>A</sup>T<sub>E</sub>X distributions — [Mik<sup>T</sup>E<sub>X</sub>](#) and [T<sub>E</sub>XLive](#) — that share lots of similarity, and L<sup>A</sup>T<sub>E</sub>X documents are portable between them. This means that, for most users, both systems are equally usable.

[T<sub>E</sub>X-Live](#) is maintained by (La)T<sub>E</sub>X developers and is certainly the best distribution you may install in your computer: However, the default distribution will take more than 5 GB on your hard disk... so, if you are not short on disk space, install T<sub>E</sub>XLive!

[Mik<sup>T</sup>E<sub>X</sub>](#) will, by default, install only a minimal set of packages. The extra/additional packages will be installed on the fly. Installing packages on the fly is useful if disk space is limited, but has its own caveats in the longer term. Definitely choose Mik<sup>T</sup>E<sub>X</sub> if you're short on disk space.

Which one to download? There are pros and cons for both distributions so it is essentially a question of where does your hear falls first! Mine is in TeXLive, but yours can be elsewhere! :D

## 2. Install L<sup>A</sup>T<sub>E</sub>X.

**Full distribution:** Installing a full distribution (valid for both TeXLive and Mik<sup>T</sup>E<sub>X</sub>) means you will have all the possibly relevant files in your computer. Almost any L<sup>A</sup>T<sub>E</sub>X file from almost any source will compile successfully in your computer.

**Basic/minimal distribution:** Installing a basic/minimal distribution (also valid for both TeXLive and Mik<sup>T</sup>E<sub>X</sub>) means your L<sup>A</sup>T<sub>E</sub>X installation will be able to compile simple documents, but you will have to add additional packages (extensions) whenever required by more complex L<sup>A</sup>T<sub>E</sub>X documents. Mik<sup>T</sup>E<sub>X</sub> makes the user's live very easy by downloading these packages automatically, while TeXLive expects the user to identify and install the required packages.

## 3. Download the novathesis template by either:

- Cloning the GitHub repository with

```
git clone --depth=1 https://github.com/joaomlourenco/novathesis.git
```

or

- Downloading the latest version from the GitHub repository as a Zip file.

## 4. Download additional School specific files if applicable:

**Universidade do Minho (UMINHO)** download the required *NewsGotT* font files from

<https://github.com/joaomlourenco/novathesis-extras/raw/main/Fonts/NewsGotT.zip>

then unzip the file and copy the 3 font files “n015002t.ttf”, “n015003t.ttf”, and “n015006t.ttf” to the folder “NOVAthesisFiles/FontStyles/Fonts”.

**Escola Superior de Enfermagem do Porto (ESEP)** download the required *Calibri* font files from

<https://github.com/joaomlourenco/novathesis-extras/raw/main/Fonts/Calibri.zip>

then unzip the file and copy the 4 font files

“Calibri.ttf”, “Calibrib.ttf”, “Calibrii.ttf”, and “Calibriz.ttf” to the folder

NOVAthesisFiles/FontStyles/Fonts.

## 5. Compile the document with you favorite LaTeX processor (pdfLaTeX, XeLaTeX or LuaLaTeX).

- The main file is named “`template.tex`”, but you are free to rename it as you please.
- Either load the main file in your favorite [LaTeX text editor](#) and press the appropriate (*magic*) button to generate a PDF file, or open a terminal and compile it with “`latexmk -pdf template`”. If you use a [L<sup>A</sup>T<sub>E</sub>X](#) text editor, please notice that the `novathesis` template uses “`biber`” and not “`bibtex`” to process the bibliography, which means that most probably you have to open the *Editor Preferences* and somewhere (depending on the Editor you are using) change “`bibtex`” to “`biber`”.
- Notice that, due to the external font sets used, `pdflATEX` will not work for both **UMINHO** and **ESEP**, and you have to use either `XELATEX` or `LuALETEX`.

6. Edit the files in the “Config” folder:

File	Contents
<code>0_memoir.tex</code>	Options specific for the memoir package. <i>Don't touch this file unless you know what you are doing!</i>
<code>1_novathesis.tex</code>	Configure the template (e.g., the document type, the school, the languages used, etc.)
<code>2_biblatex.tex</code>	Configure the bibliography.
<code>3_cover.tex</code>	Configure cover contents (e.g., author's name, thesis/dissertation title, advisers, committee, etc)
<code>4_files.tex</code>	Configure the files for chapters, appendices, annexes, abstracts, glossaries, etc...
<code>5_packages.tex</code>	Configure additional packages and commands.
<code>6_list_of.tex</code>	Configure the lists to be printed (table of contents, list of figures, list of tables, list of listings, etc). <i>Don't touch this file unless you know what you are doing!</i>
<code>9_nova_fct.tex</code>	Configuration specific to NOVA-FCT.
<code>9_nova_ims.tex</code>	Configuration specific to NOVA-IMS.
<code>9_nova_itqb.tex</code>	Configuration specific to NOVA-ITQB.
<code>9_ulisboa_fmv.tex</code>	Configuration specific to ULISBOA-FMV.
<code>9_uminho.tex</code>	Configuration specific to UMINHO (all Schools).

7. Recompile de document.

8. And you're done with a beautifully formatted thesis/dissertation! :D

### 2.2.2 With a Remote Cloud-based Service

Follow these steps to get started with a remote L<sup>A</sup>T<sub>E</sub>X installation:

- Download the [latest version from the GitHub repository as a Zip file](#).
- Login to your favorite LaTeX cloud service. I recommend [Overleaf](#) but there are alternatives. These instructions apply to Overleaf and you'll have to adapt for other providers.
- In the menu select **New project** → **Upload project**.
- Select “`template.tex`” as the main file.
- Follow from Step 5 above in Section 2.2.1 ([With a Local L<sup>A</sup>T<sub>E</sub>X Installation](#)).

## 2.3 Folder and Files

The `novathesis` template is organized into many files and folders. At the main level it includes the following files and folders listed in Table 2.1.

Table 2.1: The folders and files.

Name	Type	Access	Contents
<code>novathesis.cls</code>	<i>file</i>		The main class file.
<code>template.tex</code>	<i>file</i>		The main template file. You need to <i>compile</i> this file with one of pdfL <sup>A</sup> T <sub>E</sub> X, X <sub>H</sub> L <sup>A</sup> T <sub>E</sub> X, or LuaL <sup>A</sup> T <sub>E</sub> X to obtain the PDF file (“ <code>template.pdf</code> ”).
<code>template.pdf</code>	<i>file</i>		A possible result of applying pdfL <sup>A</sup> T <sub>E</sub> X to the “ <code>template.tex</code> ” file. The look and feel of the document will depend on the parametrization/configuration (e.g., School) of this template.
<code>Chapters</code>	<i>folder</i>		Examples of document contents, including Chapters, Appendices, Annexes, Abstracts, Glossaries, Lists of Symbols, etc. Replace them with your own.
<code>Bibliography</code>	<i>folder</i>		Where all your bibliography files should be located. You may have many as you want, as long as you add them to the template with “ <code>\ntaddfile{bib}{FILENAME.bib}</code> ”.
<code>NOVAthesisFiles</code>	<i>folder</i>		Additional files for the <code>novathesis</code> template. Unless you know what you are doing, avoid messing up with the files and folders inside this folder.

## 2.4 novathesis.cls Class Options

The `novathesis.cls` class (`novathesis.cls`) can be customized with the options listed below.

**docdegree=OPT**

*phd(\*), phdplan, phdprop, msc, mscplan,  
bsc, plain*

**The type of the document.**

phd → PhD thesis (*default*)  
 phdplan → PhD thesis plan  
 phdprop → PhD thesis proposal  
 msc → MSc dissertation  
 mscplan → MSc dissertation plan  
 bsc → BSc report  
 plain → Other report

---

**school=OPT**

*nova/fct, nova/fcsh, nova/ims,  
nova/ensp, nova/itqb, ulisboa/ist,  
ulisboa/fc, ulisboa/fmv, uminho/ea,  
uminho/ec, uminho/ed, uminho/ee,  
uminho/eeg, uminho/em, uminho/ep,  
uminho/ese, uminho/ics, uminho/ie,  
uminho/ilch, uminho/i3b, iscteiul/eta,  
ips/ests, ipl/isel, ultt/deisi, other/esep*

**The name of the school.**

This option changes the typesetting of the cover and some School specific formating, like margins, fonts, paragraph spacing and indentation, etc. . .

**lang=OPT**

*en(\*), pt*

**The main language for the document.**

Currently only Portuguese and English are supported. Other languages are expected to be support in forthcoming versions.

---

**fontstyle=OPT**

*bookman, charter, fourier, kpfonts(\*),  
mathpazo1, mathpazo2, newcent*

**The font set to be used in the document.**

Please note that a font set include definitions for the main text, headings, maths, etc.

---

**chapstyle=OPT**

*bianchi, bluebox, brotherton, dash,  
default, elegant(\*), ell, ger, hansen, ist,  
jenor, lyhne, madsen, pedersen, veelo,  
vz14, vz34, vz43*

**The chapter style**

The look of the chapter beginning.

**converlang=OPT**

*en, pt(\*)*

**The language to be used when typesetting the cover page.**

---

**otherlistsat=OPT**

*front(\*), back*

**Where to put the other lists besides the table of contents.**

The default is (front) before the main text. But some scientific areas prefer them at the end of the document (back), just before the Appendixes.

---

## 2.5. ADDITIONAL CONSIDERATIONS ABOUT THE CLASS OPTIONS

---

<b>statement=OPT</b> <i>true, false(*)</i>	<b>Include or don't include the contents of the "statement" file.</b> The default is for this file to be ignored (if it exists).
<b>linkscolor=OPT</b> <i>darkblue(*), black</i>	<b>The color for all the hyperlinks in the PDF file.</b> The "media=paper" option (see below) will override this option to "black"
<b>spine=OPT</b> <i>true, false(*)</i>	<b>Generate the book spine and the last page in the PDF.</b>
<b>biblatex=OPT</b> <i>OPT={list of options for biblatex}</i>	<b>Customize biblatex, the bibliography management system used in this class.</b> Probably you will want to change the value of the biblatex "style" option. For other customizations of biblatex check its manual.
<b>memoir=OPT</b> <i>OPT={list of options for memoir}</i>	<b>Customize the base class memoir.</b> The memoir manual should be the first document to be consulted when looking for "how can I do this?" You may want to change the base font size from 11pt to a smaller (10pt) or larger (12pt) size. Also, remember to change the "draft" to final when your document is finished.
<b>media=OPT</b> <i>screen(*), paper</i>	<b>Behavior to be customized in the school options/configuration.</b> Expected definitions for screen are: left and right margins are equal and use colored links. Expected definitions for paper are: left and right margins are different and use black links.

---

## 2.5 Additional considerations about the class options

In this section we will provide some additional considerations about some of the customizations available as class options.

### 2.5.1 The main language

The choice of the main language with the option "lang=OPT" affects:

- **The order of the summaries.** First is printed the abstract in the main language and then in the foreign language. This means that if your main language for the document is English, you will see first the "abstract" (in English) and then the

"resumo" (in Portuguese). If you switch the main language for the document for Portuguese, it will also automatically switch the order of the summaries to "resumo" and then "abstract".

- **The names for document sectioning.** E.g., "Chapter" vs. "Capítulo", "Table of Contents" vs. "Índice", "Figure" vs. "Figura", etc.
- **The type of documents in the bibliography.** E.g., "Technical Report" vs. "Relatório Técnico", "PhD Thesis" vs. "Tese de Doutoramento", etc.

No matter which language you chose, you will always have the appropriate hyphenation rules according to the language at that point. You always get Portuguese hyphenation rules in the "Resumo", English hyphenation rules in the "Abstract", and then the main language hyphenation rules for the rest of the document.

### 2.5.2 Class of Text

You must choose the class of text for the document. The available options are:

1. **bsc** — BSc graduation report.
2. **\*mscplan** — Preparation of MSc dissertation. This is a preliminary report graduate students at DI-FCT-NOVA must prepare to conclude the first semester of the two-semesters MSc work. The files specified by \ntdedicatoryfile and \acknowledgmentsfile are ignored, even if present, for this class of document.
3. **msc** — MSc dissertation.
4. **phdprop** — Proposal for a PhD work. The files specified by \ntdedicatoryfile and \acknowledgmentsfile are ignored, even if present, for this class of document.
5. **prepphd** — Preparation of a PhD thesis. This is a preliminary report PhD students at DI-FCT-NOVA must prepare before the end of the third semester of PhD work. The files specified by \ntdedicatoryfile and \acknowledgmentsfile are ignored, even if present, for this class of document.
6. **phd** — PhD dissertation.

### 2.5.3 Printing

You must choose how your document will be printed. The available options are:

1. **oneside** — Single side page printing.
2. **\*twoside** — Double sided page printing.

### 2.5.4 Font Size

You must select the encoding for your text. The available options are:

1. **11pt** — Eleven (11) points font size.
2. **\*12pt** — Twelve (12) points font size. You should really stick to 12pt...

### 2.5.5 Text Encoding

You must choose the font size for your document. The available options are:

1. **latin1** — Use Latin-1 ([ISO 8859-1](#)) encoding. Most probably you should use this option if you use Windows;
2. **utf8** — Use [UTF8](#) encoding. Most probably you should use this option if you are not using Windows.

### 2.5.6 Examples

Let's have a look at a couple of examples:

- Preparation of PhD thesis, in portuguese, with 11pt size and to be printed single sided (I wonder why one would do this!)  
`\documentclass[prephd,pt,11pt,oneside,latin1]{thesisifct-nova}`
- MSc dissertation, in English, with 12pt size and to be printed double sided  
`\documentclass[msc,en,12pt,twoside,utf8]{thesisifct-nova}`

## 2.6 How to Write Using LATEX

Please have a look at Chapter 3, where you may find many examples of LATEX constructs, such as Sectioning, inserting Figures and Tables, writing Equations, Theorems and algorithms, exhibit code listings, etc.

## 2.7 Example glossary, acronyms, and symbols

This is the first occurrence of an abbreviation: [abbreviation of a longer text \(abbrev\)](#). And now the second occurrence of the same abbreviation: [abbrev](#). And a new acronym with capital letter: [And extension of a xpto \(xpto\)](#) and reused [xpto](#). Let's also use a few other acronyms such as [acronym aaa \(aaa\)](#), [acronym aab \(aab\)](#), [acronym aba \(aba\)](#), [acronym bbb \(bbb\)](#) and [xpto](#). In geometry, the area enclosed by a circle of radius [r](#) is  $\pi r^2$ . Here the Greek letter [π](#) is equal to the ratio of the circumference of any circle to its diameter.

## CHAPTER 2. NOVATHESIS TEMPLATE USER'S MANUAL

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Lets add “[computer](#)” to the glossary! Be carefull with mathematical symbols in acronyms, please see the definition of [Mu \( \$\mu\$ \)](#).

Reference to Potassium  $K^+$  and Sodium  $Na^+$  as well.

---

# A Short L<sup>A</sup>T<sub>E</sub>X Tutorial with Examples

This Chapter aims at exemplifying how to do common stuff with L<sup>A</sup>T<sub>E</sub>X. We also show some stuff which is not that common! ;)

Please, use these examples as a starting point, but you should always consider using the *Big Oracle* (aka, [Google](#), your best friend) to search for additional information or alternative ways for achieving similar results.

## 3.1 Document Structure

## 3.2 Dealing with Bibliography

Citing something online [4, 6, 8].

## 3.3 Inserting Tables

## 3.4 Importing Images

## 3.5 Floats, Figures and Captions

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

Nulla malesuada porttitor diam. Donec felis erat, congue non, volutpat at, tincidunt tristique, libero. Vivamus viverra fermentum felis. Donec nonummy pellentesque ante. Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo. Maecenas lacinia. Nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem. Sed lacinia nulla vitae enim. Pellentesque tincidunt purus vel magna. Integer non enim. Praesent euismod nunc eu purus. Donec bibendum quam in tellus. Nullam cursus pulvinar lectus. Donec et mi. Nam vulputate metus eu enim. Vestibulum pellentesque felis eu massa.

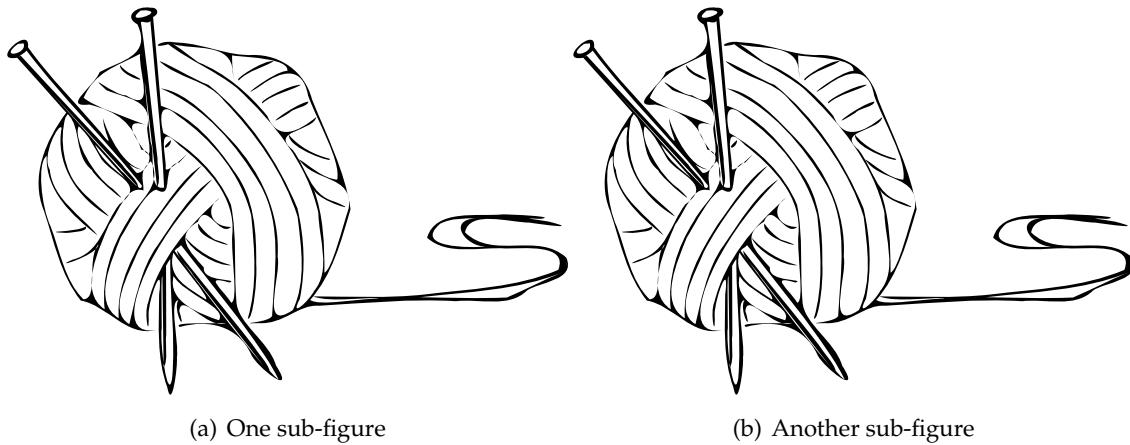


Figure 3.1: A figure with two sub-figures!

**And this is a small text that references the Figure 3.1 and its Subfigures 3.1(a) and 3.1(b).**

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan

eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

Nulla malesuada porttitor diam. Donec felis erat, congue non, volutpat at, tincidunt tristique, libero. Vivamus viverra fermentum felis. Donec nonummy pellentesque ante. Phasellus adipiscing semper elit. Proin fermentum massa ac quam. Sed diam turpis, molestie vitae, placerat a, molestie nec, leo. Maecenas lacinia. Nam ipsum ligula, eleifend at, accumsan nec, suscipit a, ipsum. Morbi blandit ligula feugiat magna. Nunc eleifend consequat lorem. Sed lacinia nulla vitae enim. Pellentesque tincidunt purus vel magna. Integer non enim. Praesent euismod nunc eu purus. Donec bibendum quam in tellus. Nullam cursus pulvinar lectus. Donec et mi. Nam vulputate metus eu enim. Vestibulum pellentesque felis eu massa.

## 3.6 Text Formatting

## 3.7 Generating PDFs from L<sup>A</sup>T<sub>E</sub>X

### 3.7.1 Generating PDFs with pdflatex

You may create PDF files either by using `latex` to generate a DVI file, and then use one of the many DVI-2-PDF converters, such as `dvipdfm`.

Alternatively, you may use `pdflatex`, which will immediately generate a PDF with no intermediate DVI or PS files. In some systems, such as Apple, PDF is already the default format for L<sup>A</sup>T<sub>E</sub>X. I strongly recommend you to use this approach, unless you have a very good argument to go for `latex + dvipdfm`.

A typical pass for a document with figures, cross-references and a bibliography would be:

```
$ pdflatex template  
$ bibtex template  
$ pdflatex template  
$ pdflatex template
```

You will notice that there is a new PDF file in the working directory called `template.pdf`. Simple :)

Please note that, to be sure all table of contents, cross-references and bibliographic citations are up-to-date, you must run `latex` once, then `bibtex`, and then `latex` twice.

### 3.7.2 Dealing with Images

You may process the same source files with both `latex` or `pdflatex`. But, if your text include images, you must be careful. `latex` and `pdflatex` accept images in different (exclusive) formats. For `latex` you may use EPS ou PS figures. For `pdflatex` you may use JPG, PNG or PDF figures. I strongly recommend you to use PDF figures in vectorial format (do not use bitmap images unless you have no other choice).

### 3.7.3 Creating Source Files Compatible with both `latex` and `pdflatex`

Do not include the extension of the file in the `\includegraphics` command. E.g., use

`\includegraphics{sonwman}`

and not

`\includegraphics{sonwman.eps}`.

If you use the first form, `latex` or `pdflatex` will add an appropriate file extension.

This means that, if you plan to use only `pdflatex`, you need only to keep (preferably) a PDF version of all the images. If you plan to use also `latex`, then you also need an EPS version of each image.

## To be included in the sections above

Para fazer citações, deverá usar-se a chave da referência no ficheiro BibTeX. Se for uma única referência [2], usar um “~” para ligar o `\cite{...}` à palavra que o precede (`... referência~\cite{Artho04}`). Caso queira fazer múltiplas citações [12, 13, 11], deverá agrupá-las dentro de um único `\cite{...}`.

Note que o ficheiro de bibliografia pode ter tantas entradas quantas quiser. Apesar das aquelas cuja chave seja referenciada no texto é que serão incluídas na listagem de bibliografia.

Footnotes<sup>1</sup> will be numbered and shown in the bottom of the page.

A Tabela 3.1 ilustra alguns conceitos importantes associados à construção de tabelas:

- i) Não usar linhas verticais;
- ii) A legenda deve ficar por cima da tabela;
- iii) Usar as macros `\toprule`, `\midrule` e `\bottomrule` para fazer a linha horizontal superior, interiores e inferior, respectivamente.

Table 3.1: Test results summary.

Test	Anomalies	Warnings	Correct	Categories	Missed
Connection [3]	2	2	1	C	1
Coordinates'03 [1]	1	4	1	2B, 1C	0
Local Variable [1]	1	2	1	A	0
NASA [1]	1	1	1	—	0
Coordinates'04 [2]	1	4	1	3C	0
Buffer [2]	0	7	0	2A, 1B, 2C, 2D	0
Double-Check [2]	0	2	0	1A, 1B	0
StringBuffer [7]	1	0	0	—	1
Account [14]	1	1	1	—	0
Jigsaw [14]	1	2	1	C	0
Over-reporting [14]	0	2	0	1A, 1C	0
Under-reporting [14]	1	1	1	—	0
Allocate Vector [9]	1	2	1	C	0
Knight Moves [3]	1	3	1	2B	0
Total	12	33	10	5A, 6B, 10C, 2D	2

As figuras a inserir no documento deverão ser de qualidade, preferencialmente em formato vectorial (PDF vectorial) e não em *bitmap* (PNG, JPG, etc). As imagens *bitmap* (Figura 3.2) não escalam bem e têm reflexos negativos na qualidade do seu documento. Pelo contrário, as imagens *vectoriais* Figura 3.3 escalam muito tanto quanto o necessário sem degradar a qualidade da imagem.

<sup>1</sup>This is a simple footnote.

Só deve usar *screenshots* se não tive mesmo nenhuma alternativa. Em vez e gerar um *screenshot*, tente usar uma impressora virtual PDF e imprimir para um ficheiro PDF. Regra geral obterá um PDF vetorial. Mesmo que o seu PDF contenha imagens, elas terão sempre qualidade maior ou igual à que obteria com um *screenshot*.

Para agregar várias figuras numa única... Poderá assim referenciar o conjunto como Figura 3.4 ou as sub-figuras separadamente como 3.4() e 3.4(a).

## 3.8 Equações

O LaTeX é uma ferramenta poderosa para escrever em estilo matemático. Permite inserir fórmulas no meio do texto como por exemplo esta:  $ax^2 + bx + c = 0$ . Também permite que as fórmulas sejam destacadas numa linha separada e centradas na página

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$
$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

ou numeradas

$$aaa \tag{3.1}$$

que depois pode ser referida no texto como sendo a equação 3.1

$$aa$$

$$a \tag{3.2}$$

$$b \tag{3.3}$$

$$c \tag{3.4}$$

$$(3.5)$$

## 3.9 Test for listings

Testing the package “listings”...

Testing the package “minted”...

Blah...

## 3.10 Test for algorithms

Uncomment the algorithms source below and add the following to file “5\_packages.tex”

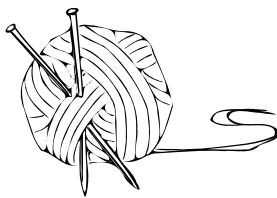
```
\usepackage{algorithm2e}
\RestyleAlgo{ruled}
```



Figure 3.2: Imagem em formato *bitmap* (JPG)



Figure 3.3: Imagem em formato PDF vectorial



(a) Novelo de lã



(b) Tempestade com neve

Figure 3.4: Exemplo de utilização de *subbottom*

and uncomment

```
\ntaddlistof{listofalgorithms}
```

in file “`8_list_og.tex`”.

---

## Bibliography

- [1] C. Artho, K. Havelund, and A. Biere. *High-Level Data Races*. 2003. URL: [citeseer.ist.psu.edu/artho03highlevel.html](http://citeseer.ist.psu.edu/artho03highlevel.html) (cit. on p. 23).
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# APPENDIX A

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## ***NOVAthesis covers showcase***

This Appendix shows examples of covers for some of the supported Schools. When the Schools have very similar covers (e.g., all the schools from Universidade do Minho), just one cover is shown. If the covers for MSc dissertations and PhD thesis are considerable different (e.g., for FCT-NOVA and UMinho), then both are shown.

## Appendix 2 Lorem Ipsum

This is a test with citing something [5] in the appendix.

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## APPENDIX B. APPENDIX 2 LOREM IPSUM

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## Annex 1 Lorem Ipsum

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## ANNEX I. ANNEX 1 LOREM IPSUM

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# 2023 X-ray Imaging Research Program Report

This report summarizes the findings of the 2023 X-ray Imaging Research Program, which focused on the development of advanced imaging techniques and their applications in various fields. The program was organized by the International Society for X-ray Imaging (ISXI) and involved researchers from around the world.

The report begins with an introduction to the program's objectives and methodology. It then provides a detailed overview of the research findings, organized into several key areas:

- Advanced Imaging Techniques:** This section discusses the development of new imaging methods, including Compton scattering imaging, phase contrast imaging, and tomographic reconstruction algorithms.
- Medical Applications:** The report highlights the potential of X-ray imaging in medical diagnostics, such as early cancer detection and non-invasive monitoring of patient health.
- Industrial Applications:** The program explored the use of X-ray imaging in quality control, materials science, and industrial process monitoring.
- Environmental Monitoring:** Researchers investigated the use of X-ray imaging for environmental monitoring, including the detection of pollutants and the study of geological processes.
- Astro-Imaging:** The report also covers the application of X-ray imaging in astrophysics, particularly in the study of black holes and other celestial bodies.

The report concludes with a summary of the program's impact and future directions, emphasizing the importance of continued research and collaboration in the field of X-ray imaging.