

For the last part of the Computational Research Techniques, you are tasked to carry out individual projects.

Everyone will have a slightly different project, in its execution similar to the one from Session 3. The projects will be allocated and discussed during Session 4 on Friday 9th of February.

You will carry out your project independently over Week 5, **submitting the report on Friday 16th of February**.

The project report is in the form of a short PDF (see templates provided), describing your project, methodology, and observations and featuring a rendering of your system and a figure plotting the analyzed quantity.

Guidance for the Report

[Marked out of total 30 pts]

Title – descriptive, direct, concise, and should not be misleading.

Overview (max. 100 words):

[5 pts]

Briefly describe the problem. What did you investigate, which approach did you use and what were the key findings and observations?

Methodology (max. 500 words):

[12 pts]

Describe all key steps in a condensed form. This section should include the minimal necessary information for someone who reads it to be able to reproduce your results.

As a guidance, include the following:

- **System setup.** Consider the following questions:
 - where did you get the structure(s) from?
 - how did you manipulate them to obtain the model you used in the simulation?
 - which forcefield(s) did you use?
 - what was your system size?

- **Simulation protocol.** Include all relevant run information for your energy minimization, equilibration, and production runs, e.g.:
 - run type algorithm (energy minimization or molecular dynamic?)
 - time step
 - simulation length
 - temperature control (thermostat)
 - pressure control (barostat)
- **Analysis.** Consider the following questions when writing this section:
 - how did you make sure your system was equilibrated within the time frame that you analyzed?
 - what analysis did you perform on your trajectories?
 - what part of the trajectory did you use? Any timeframes skipped?
 - include all relevant information about the analysis you performed on your trajectories, software (e.g., GROMACS, VMD), and tools within those you used (e.g., gms density, gms rms, etc.); which parameters did you use when running these analysis tools.
 - how did you prepare the plot of your analysis data?
 - how did you produce the rendering of your system?

Results (max. 400 words, incl. figure captions):

[Total 13 pts, incl. 5 pts for figures, 3 pts for captions]

Describe your result data with a plot that illustrates your findings and a rendering of the system, highlighting a key interaction or alignment. Make sure to add all the descriptive captions that are necessary for understanding the figures without the need to refer to the text.

References (not included in word count):

Include consistently formatted references for relevant literature, structures, forcefield parameters, and software packages used in your project.

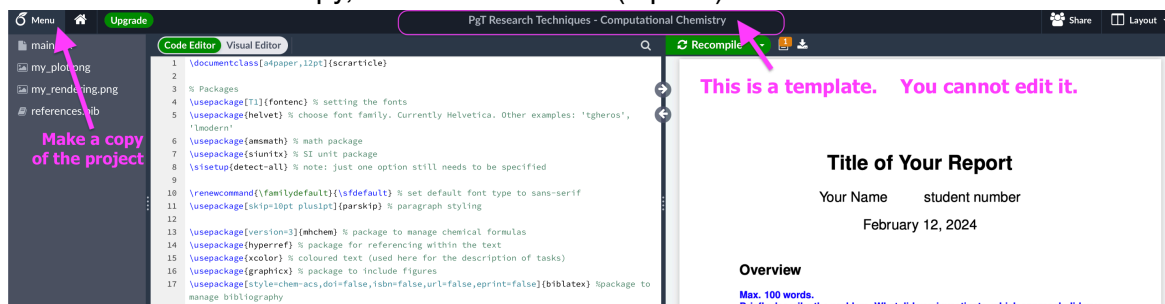
Project Report Templates

The project should be submitted as a PDF file. We encourage you to use one of the following two templates to guide you through report preparation.

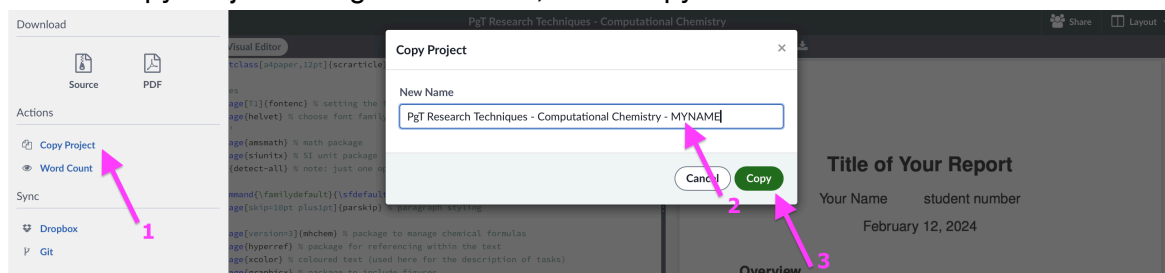
- Word .doc template [TemplatePgTResearchTechniques_CompChem.dotx](#)
- OverLeaf LaTeX template (we will discuss how to use OverLeaf during session 4) [Link to](#)

Using OverLeaf Template:

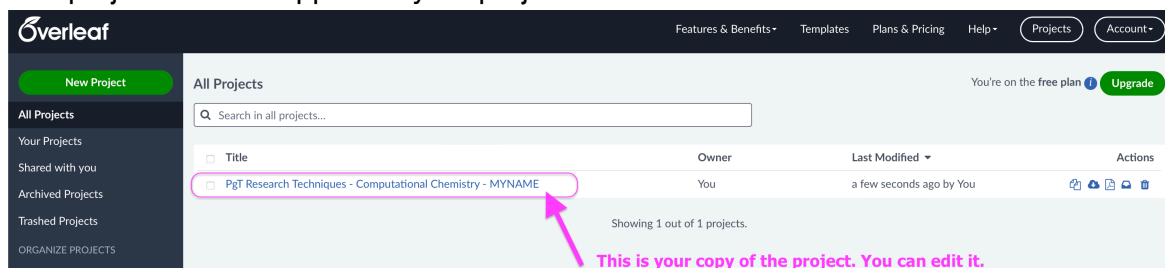
1. Register with your University email at [Overleaf.com](#)
2. Click on the link to the [OverLeaf Template](#); you will be prompted to 'Join the Project', click yes, and it will open in your browser.
3. This is a template and is not editable.
4. To make an editable copy, click on the 'Menu' (top left)



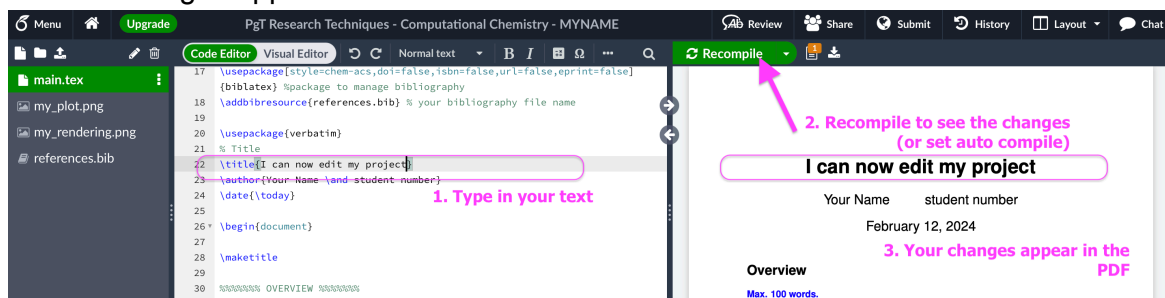
5. Select 'Copy Project' and give it a name, click 'Copy'



6. The project will now appear in your project list



7. Click on the project to open it. You can now edit the text. Make sure to click compile to see the changes appear on the PDF



8. When you are ready to submit, you can download a PDF (make sure to do a final recompile!)

Download

Source PDF

Actions

- Copy Project
- Word Count

Sync

- Dropbox
- Git
- GitHub

Research Techniques - Computational Chemistry - MYNAME

Visual Editor

Recompile

My amazing project

Nelle Scientist S123456

February 12, 2024

Overview

This is my first CompChem project. I also learned how to write it using LaTeX in OverLeaf template. I should be proud of all I have learned over the last few weeks and the achievements I have made!

When ready, download the PDF for submission:
- Click 'Menu' (top left)
- Click 'PDF' (the pdf will appear on your computer in your standard 'Downloads' folder)