Report and code outline

Digital Chemistry FS24 project

The **report** is expected to be between 4-5 pages, with supplementary material in the Appendix. It should consist of the following sections:

Introduction

This section should contain a brief introduction about the topic of the project and its relevance (1-2 paragraph(s)). Additionally, it should clearly state the goal of the project.

Methods

This section should contain a detailed description of the workflow and methodology applied to achieve the described goal. Choices within the project, e.g. model selection and validation, have to be explained in this section. This section should contain one figure which gives an overview of the workflow of the project.

Results and Discussion

This section should contain a brief description of the main results of the project as well as interpretation and discussion of them. In particular, benefits and limitations should be identified and described. Results should be presented in figures and tables that are discussed in the text. Additional results that are relevant but not central to the discussion can be put in an appendix.

Outlook

A brief outlook on the project about the applicability of the project in a broader context and the improvement of the project should be presented.

One-sentence summaries

One-sentence summaries for each of the following points should be provided:

- Problem/Task
- Approach
- Results and Impact
- Challenges and Future Work

Lastly, a confirmation has to be provided, signed by every student who participated in the project, confirming they contributed to the project and agree with the handed-in documents. Digital signatures are also accepted.

In addition to the report, the code has to be provided to the teaching team. The preferred way of providing the code is through git, either GitHub or GitLab. For the latter, ETH has a server. Even though it is not required, if you and your group want to work collaboratively using git, you can find an introduction here. Alternatively, feel free to contact the teaching team with any inquiries. Otherwise, you can develop your code not using GitHub / GitLab and upload the required files in the end for the submission. An introduction for doing this on GitLab can be found below.

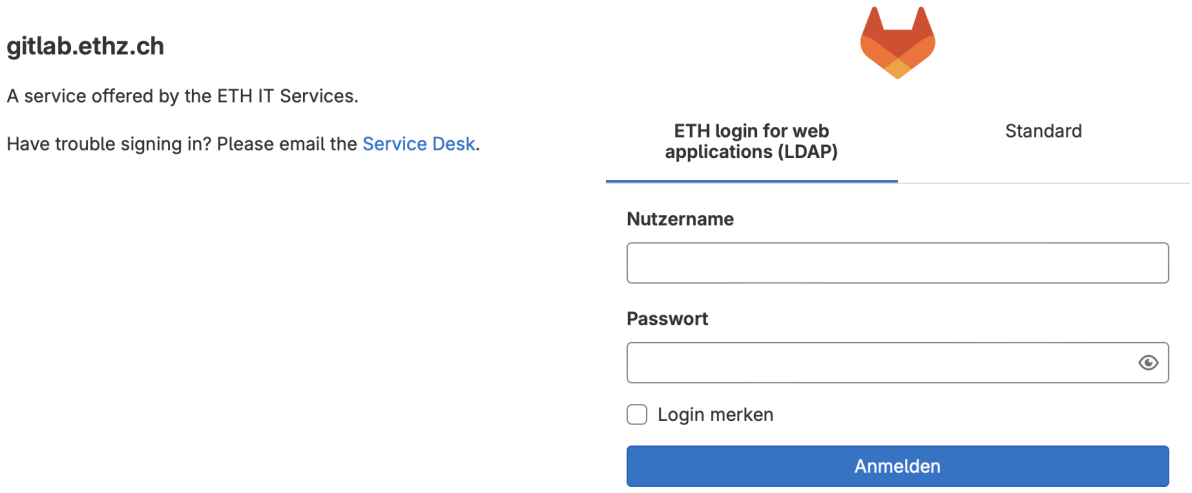
The provided material has to contain the following:

- The report.
- All of the required code for the project.
- One or multiple files to reproduce the results. This can also be downloaded from Google Colab if you work with Google Colab.
- A README file which contains a description of what is in the provided files.
- In case you did not complete your project in Google Colab, provide an environment.yml or requirements.txt file from your coding environment.

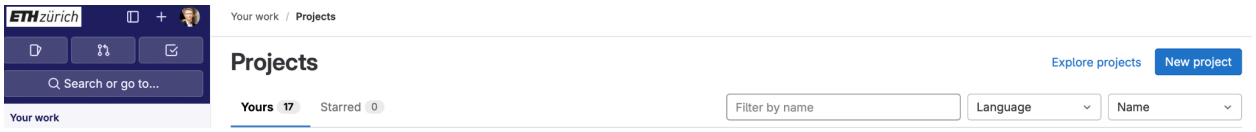
Introduction to upload files in GitLab for final submission:

Below you see an introduction on how to create a new project on Gitlab, upload your files to the project and share it with the teaching team. This can be used to submit your project when you have not used GitHub or GitLab for your project. The presence of this introduction should not discourage you from using git for your project.

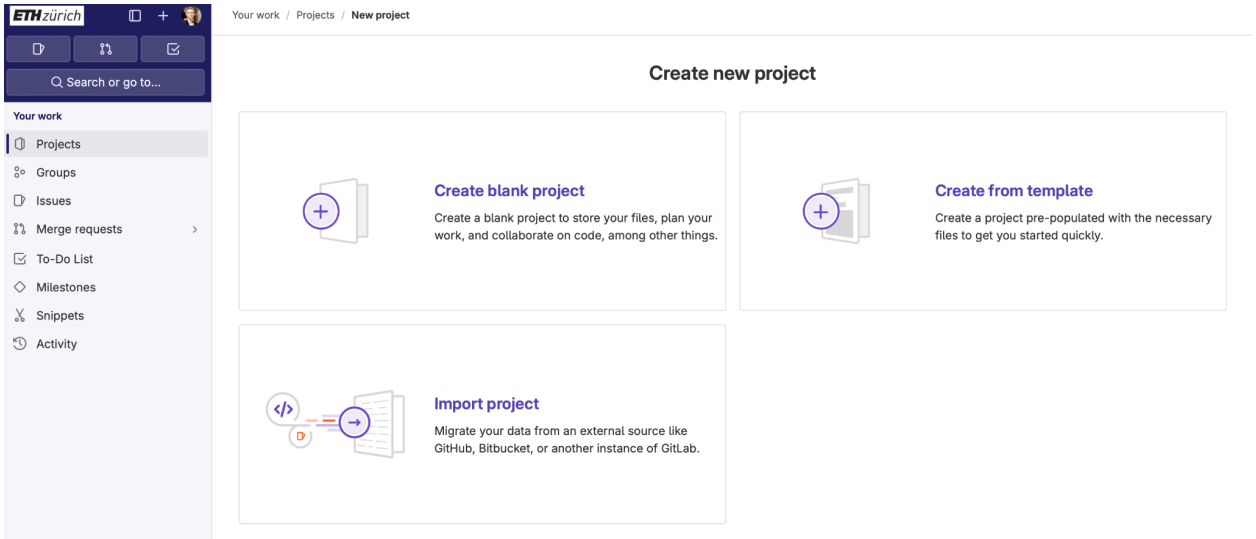
1. Go to gitlab.ethz.ch and log in with your ETH account



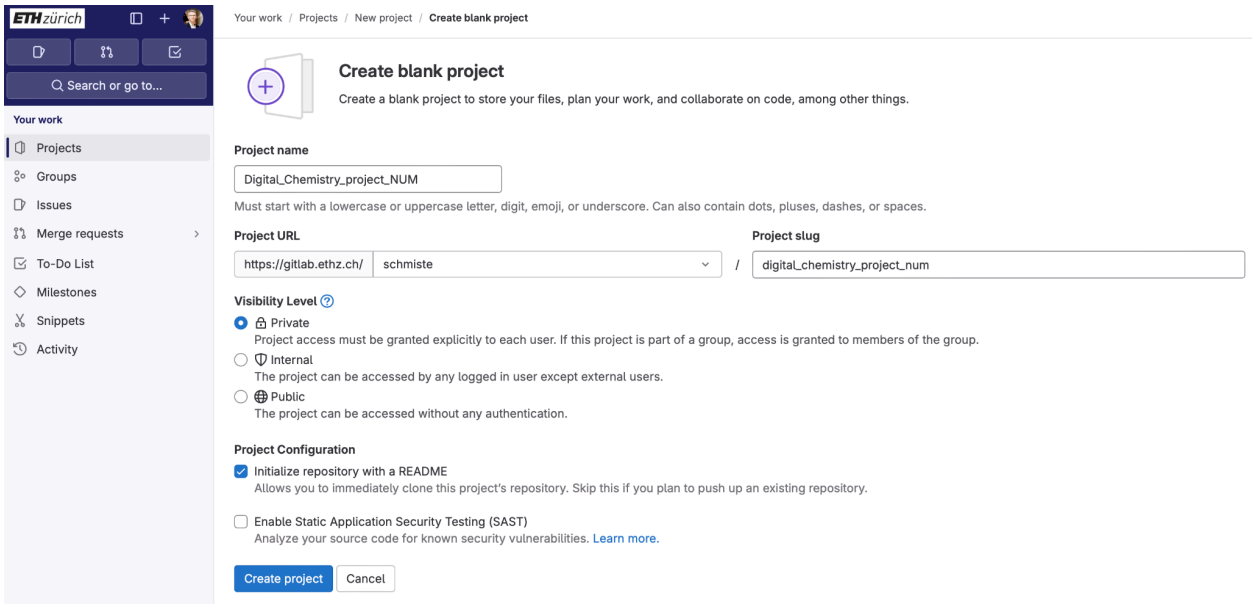
2. After you logged in, create a new project on the top right



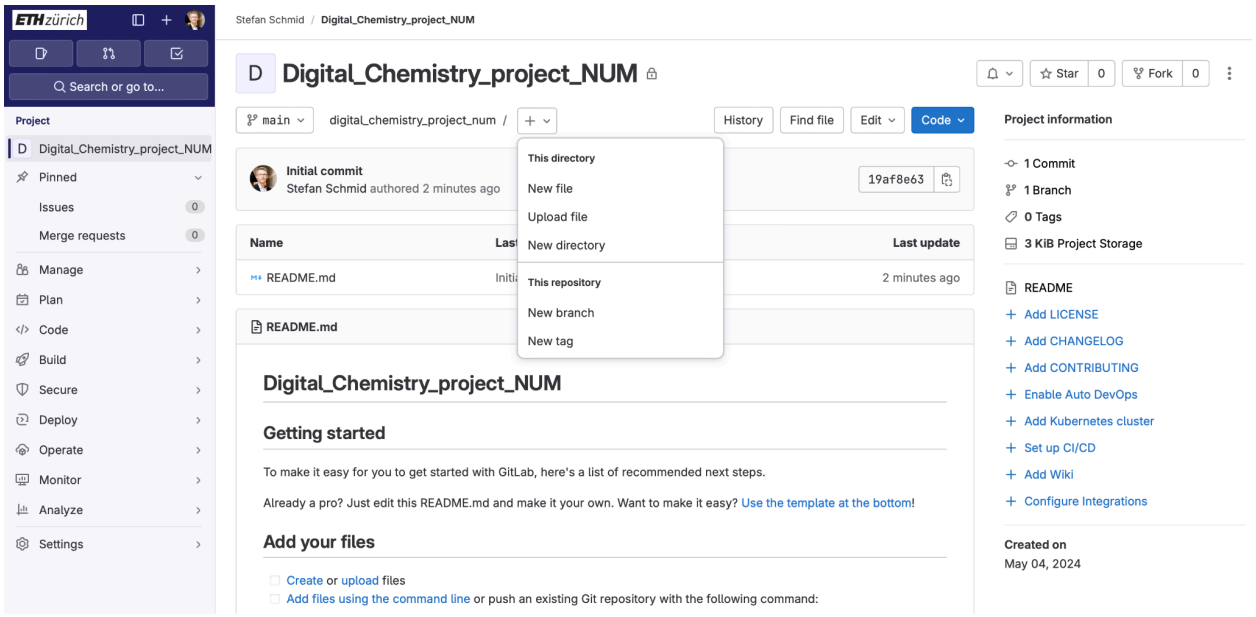
3. Create a blank project



4. Give the project an informative name; one example could be to name it *Digital_Chemistry_project_NUM*, where NUM is the number of your project; set the visibility level to private and click on create project



5. Click on the +-sign and select upload files to upload the files you want to submit



6. Lastly, for final submission, add the teaching team to the project. Do this by clicking on Manage > Members on the right column and then add the teaching team with the following user names:

   Kjell Jorner: kjorner; Stefan: schmiste; Lauriane: laurianejd;