


---

# Computing Methods in Particle Physics

Karolos Potamianos, Elisabeth Schopf  
February/March 2022



The lecture slides and content are heavily based on what originally has been put together by Matthew Bass and modified by Giacomo Artoni.  
Huge credit goes to them!

# Lecture Overview

---

## 1. Introduction - today

- a. Commonly used computing tools
- b. Setting up the computing environment for this course
- c. Python, numpy, matplotlib examples

## 2. Bayesian Inference & Fitting

## 3. Classification problems & machine learning

## 4. Deep Learning

Each lecture will have some slides + practical, hands-on examples

→ Aims: Introduce a broad range of computing concepts and tools commonly used in particle physics with a focus on machine learning. We can't possibly cover everything in this lecture but hope to give an overview and starting point for more in depth studies.

# Materials and contact

---

For any questions feel free to contact us: [karoos.potamianos@cern.ch](mailto:karoos.potamianos@cern.ch),  
[elisabeth.schopf@cern.ch](mailto:elisabeth.schopf@cern.ch)

All lecture material can be found here: <https://gitlab.com/oxford-physics/cmpp>

Further reading:

- “Effective Computation in Physics”, A. Scopatz, K. D. Huff
- [Frequentism and Bayesianism: A Python-driven Primer](#)
- [HSF analysis essentials](#) for HEP data analysis
- [TMVA user's guide](#)
- [scikit-learn user's guide](#)

# Particle Physics and Programming

---

In particle physics you are most likely working with large data sets and collaborating with others → efficient data handling, analysis and collaborative software development are key!

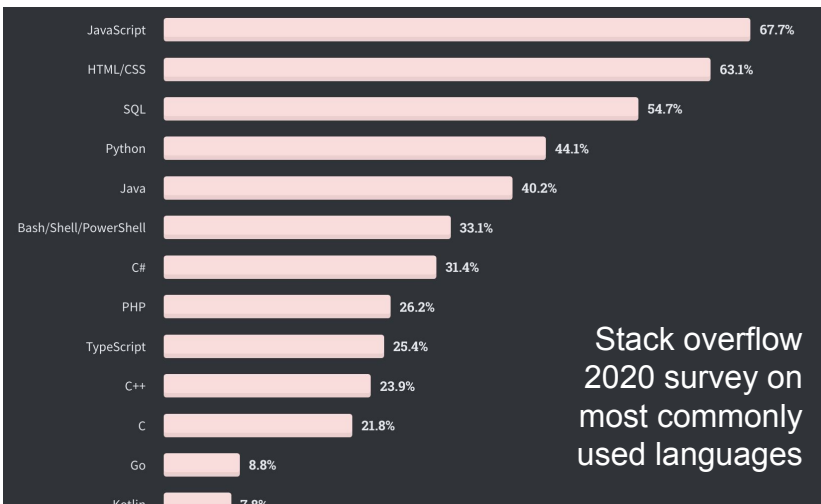
Tools you likely will use in one way or another:

- Programming languages
- Linting & debugging
- Shell environments & shell scripts
- Plotting tools
- Data management tools
- Version control
- Build systems

# Programming Languages and Coding

# Most commonly used languages

There is a breadth of programming languages out there. In particle physics (analysis) C++ and python are most commonly used. In technical settings you might also encounter others (java, SQL, etc.)



Stack overflow  
2020 survey on  
most commonly  
used languages

+ ...

## ATLAS reconstruction software



athena

Project ID: 53790

☆ Star 159

90,469 Commits 36 Branches 2,448 Tags 153.2 MB Files 727.3 MB Storage 244 Releases

The ATLAS Experiment's main offline software repository

DOI 10.5281/zenodo.2641997

68.4% C++

26.0% Python

For data analysis at the end of the chain, i.e. after reconstruction, pre-processing of the data, [python](#) is becoming increasingly popular

- Python requires no extra compilation step
- It interfaces to many external libraries easily, e.g. ROOT, sci-kit learn, etc.

You will likely share your code and its development with others and need to rerun pieces of code after many months/years of not using them, e.g. re-running plots for your thesis → Reminder of best practices (not only for python):

- **Give variables/functions sensible, self-explanatory names**
- **Take the time to write comments in the code**



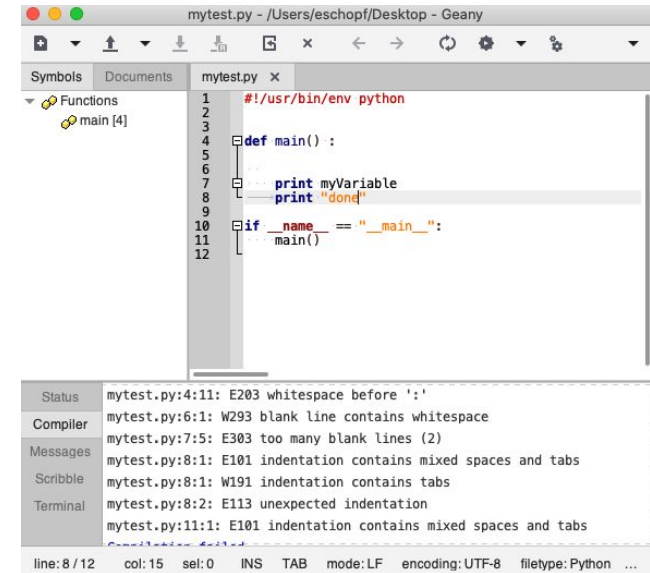
# Tools for inspecting your code: lint & syntax check

A linter checks your code for **coding style issues** → helps to maintain good readability of the code and cross-editor compatibility

Most editors - geany, emacs, etc. - come with built in linters

Many editors also allow you to **check code syntax for errors**

- **Attention:** depending on compiler environment and language version the errors/suggestions you get locally in your editor might not be the same as in your final environment
- **Good practice to always test the code in the place where it is intended to run!**



```
1 #!/usr/bin/env python
2
3
4 def main() :
5
6
7     print myVariable
8     print "dond"
9
10 if __name__ == "__main__":
11     main()
12
```

Status	Message
Compiler	mytest.py:4:11: E203 whitespace before ':'
Compiler	mytest.py:6:1: W293 blank line contains whitespace
Compiler	mytest.py:7:5: E303 too many blank lines (2)
Messages	mytest.py:8:1: E101 indentation contains mixed spaces and tabs
Scribble	mytest.py:8:1: W191 indentation contains tabs
Terminal	mytest.py:8:2: E113 unexpected indentation
Terminal	mytest.py:11:1: E101 indentation contains mixed spaces and tabs

line: 8 / 12 col: 15 sel: 0 INS TAB mode: LF encoding: UTF-8 filetype: Python ...

# Tools for inspecting your code: debuggers

---

Debuggers can be very powerful tools to **inspect the logic of your code and help finding unexpected errors or output**

A debugger allows to step through the code line by line, evaluate expressions at each point in the code, etc.

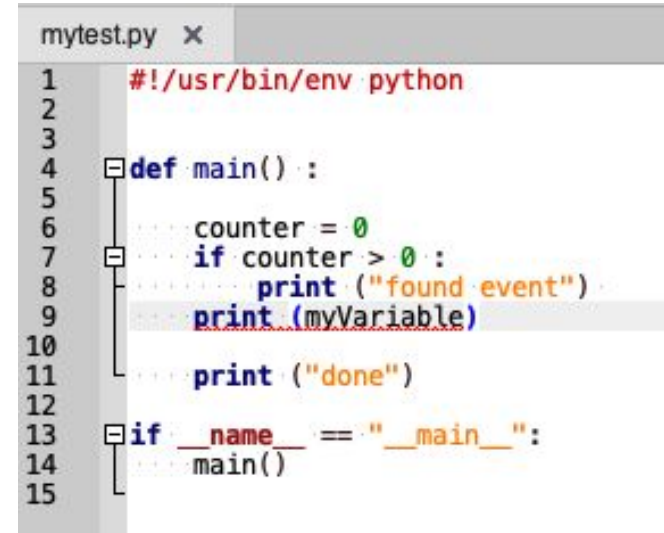
- Some editors come with built in debuggers
- Python also has its own debugger [pdb](#) that comes with (most) python installations
- For C++ use, e.g. [gdb](#)

# Debugging example

```
(base) eschopf@ppmac1ap01 Documents % python -m pdb ~/Desktop/mytest.py
> /Users/eschopf/Desktop/mytest.py(4)<module>()
-> def main() :
(Pdb) step
> /Users/eschopf/Desktop/mytest.py(13)<module>()
-> if __name__ == "__main__":
(Pdb) step
> /Users/eschopf/Desktop/mytest.py(14)<module>()
-> main()
(Pdb) step
--Call--
> /Users/eschopf/Desktop/mytest.py(4)main()
-> def main() :
(Pdb) step
> /Users/eschopf/Desktop/mytest.py(6)main()
-> counter = 0
(Pdb) step
> /Users/eschopf/Desktop/mytest.py(7)main()
-> if counter > 0 :
(Pdb) p counter
0
(Pdb) step
> /Users/eschopf/Desktop/mytest.py(9)main()
-> print (myVariable)
```

Stepping through  
the code

Evaluate value of  
counter



```
mytest.py x
1  #!/usr/bin/env python
2
3
4  def main() :
5
6      counter = 0
7      if counter > 0 :
8          print ("found event")
9          print (myVariable)
10
11         print ("done")
12
13  if __name__ == "__main__":
14      main()
15
```

# Tools for inspecting your code: profiling

---

If performing millions of time, computing and memory extensive operations

- Processing millions of data events
- Applying complex corrections
- Handling multiple copies of objects
- ...

it might be useful to understand **which parts of the code consume most resources** to potentially optimise in that regard

There are open source tools available, e.g. [valgrind](#), to do so

# Version control: keeping track of code developments

---

Version control tracks and integrates changes to your code. In its core it allows to:

- Keep track of changes made by providing some form of change log/history
- Integrate (“merge”) code changes into existing code
- Revert changes or go back to previous code versions
- Create version tags of the code in a specific point in time/development

For common code and code used to produce public results version control is **a must to ensure reproducibility and be able to recall the logic that went into developing** the analysis.

Keeping your personal code under version control is a good habit too!

# Version control software

---

One of the most popular version control softwares is git:

- [Github](#) is a popular place to host software
- [Gitlab](#) is another one and extensively used for [CERN based projects](#)

Other version control software are svn, bazaar, etc.



# Build systems

---

Complex (C++ based) analysis frameworks often require a **build system that manages the compilation and takes care of dependencies and environment setups**.

It also handles software version requirements, cross-platform issues, etc.

On a small scale often having a **Makefile** is sufficient for more complex software build systems like **CMake**, **CMT**, **MRB**, etc. are available

Usually your experiment's software tools come with their build system and you probably don't need to set it up yourself

# Data Handling and Visualisation



**Experiments all have their specific data management strategy** - mostly centered around ROOT.

In most cases data is provided in an already pre-processed and machine readable format and you will just perform specific higher-level tasks on them and visualise the output.

In cases where you need to process raw data yourself or produce simulations you can in most cases follow your experiment's recipes (and in an ideal case: tutorial)

- **Metadata is important for reproducibility** since it keeps track of what happened to the data, which software versions it was processed with, etc.

# Data Management Tools

---

The general idea of all data management tools is to **store data in a table-like format while preserving relationships** between fields

Many database tools/languages available: SQL (popular in industry), Pandas (for python), etc.

ROOT (often used in particle physics):

- TTree class with branches to store data (ints, floats, etc., but also vectors or physics objects as implemented by ROOT, e.g. TLorentzVector)
- Storage of custom C++ objects (e.g. reconstructed “Electron” objects)
- Storage of analysis objects (histograms, canvases)

It is useful to know other ones than ROOT because for interfacing to external tools, e.g. machine learning tools, it is sometimes necessary to convert data back and forth

# Shell Scripts

Easy way to **automate simple, repetitive tasks**, like:

- Executing a sequence of commands, e.g. setting up your environment
- Renaming/copying files following a specific pattern
- Submitting jobs to a batch system
- ...

and allows to interact with Unix & experiment specific tools. Often faster than writing and executing a python script

Most common scripting language: **Bash** (also common zsh)

```
1  #!/bin/bash
2
3  ID=0
4
5  # make your life easier by not typing out long strings
6  if [ $ID = 0 ]
7  then
8      IDSTRING="AnalysisZero"
9  elif [ $ID = 1 ]
10 then
11     IDSTRING="AnalysisOne"
12 fi
13
14 # do something with files in specific cases
15 if [ $ID == 0 ]
16 then
17     rm ${IDSTRING}.*categoryXY*.txt
18 fi
19
20 # do something with files
21 for file in ${IDSTRING}*.txt
22 do
23     cat $file >> allData.txt
24 done
25
26
```

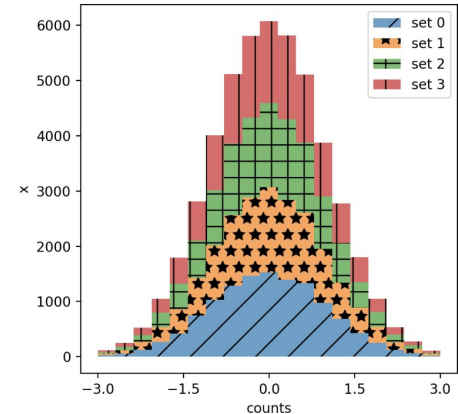
# Plotting Tools

There are ample tools available to visualise data!

Which one is most convenient to use might also depend on the format your data is provided in and existing tools (however, it's always good to know what's out there)

- [ROOT](#): very common in particle physics; pyROOT interfaces to python
- [Matplotlib](#): visualisation library designed for python
- [Gnuplot](#): command line driven visualisation tool
- ...

All of them offer wide range of plotting types and options



Provides a wide array of functionalities tailored towards particle physics needs:

- Plotting (e.g. TH1 - 1D histograms, TGraph - graphs, etc.)
- Data management (e.g. TTree)
- Commonly used objects (e.g. TLorentzVector - four momentum vectors), mathematical functions (see e.g. TF1 formula class) and operations
- Fitting (RooFit)
- GUI (see TBrowser)
- Machine learning (see TMVA class)

It is possible to install ROOT on your computer; if you are running on a particle physics computing cluster (e.g. Oxford [PPUnix](#) or CERN [lxplus](#)) most likely it is already installed there

# Summary

---

There are lots of open source computing tools and languages available to analyse, handle and visualise data; which one is best to use often depends on what you want to achieve and general practices in your experiment

How to get started on a project:

- Think about your data sources and analysis needs
- Setup version control or check-out and setup version controlled experiment specific framework
- Make sure to document (in-line comments, READMEs, docstring for python, doxygen, etc.)
- Start coding and make frequent commits

# Setting up your Environment for this Course

# Operating systems and computing environments

---

Any - Windows, Linux, MacOS - will work for this course and data analysis in general.

If specific software requires a specific operating system it is possible to virtually run it (virtual machines/emulators), e.g. [VirtualBox](#) a virtual machine host tool

If you don't want to pollute your computer with software or run a virtual machine you might also choose to not work on your computer directly but instead:

- ssh to Oxford's or your experiment's/lab's computing cluster
- Work on an online hosted computing environment, e.g. [google colab](#), [CERN Swan](#), etc.



# Suggested exercises for today's lecture

---

1. Set-up your computing environment (see next slides)
  - a. It is always good to have a minimal working (python) set-up on your computer
  - b. For this course we will mostly use jupyter workbooks, which will not run from the PPUX or Ixplus computing clusters
  - c. For this course we have at least one example with ROOT, which requires connection to PPUX
2. Get the matplotlib, numpy and pandas examples and check if they are working in your setup
3. Set-up a github/gitlab account (if you don't have one yet) and create a new project for this lecture to house your jupyter notebooks and changes
4. Get familiar and play around with these examples and tools :-)

Do not hesitate to ask in case something is unclear or not working and we will try to help!

# Set-up for your computer: installing python

---

Check if python is already installed, e.g. type in your terminal `which python` (if yes, you can type `python -V` to get the python version number you are using)

If you need to install python, would like to update to a newer version or add python libraries that are not part of the default installation:

- “Raw” installation directly from python ([Linux](#), [Windows](#), [Mac](#)) and add packages by e.g. downloading from gitlab (**not recommended**)
- Using an installation environment that also can help downloading additional python libraries and takes care of dependencies, e.g.:
  - [Anaconda](#)\*
  - [Homebrew](#)
  - [pip](#)\* (needs existing python installation but comes by default with newer python versions)

\*I can personally recommend

# Adding additional packages/libraries to python

---

Useful things to add for this course (and also in general):

```
numpy scipy ipython ipython-notebook matplotlib pandas pytables  
nose setuptools sphinx mpi4py seaborn pymc pymc3
```

They can be installed via:

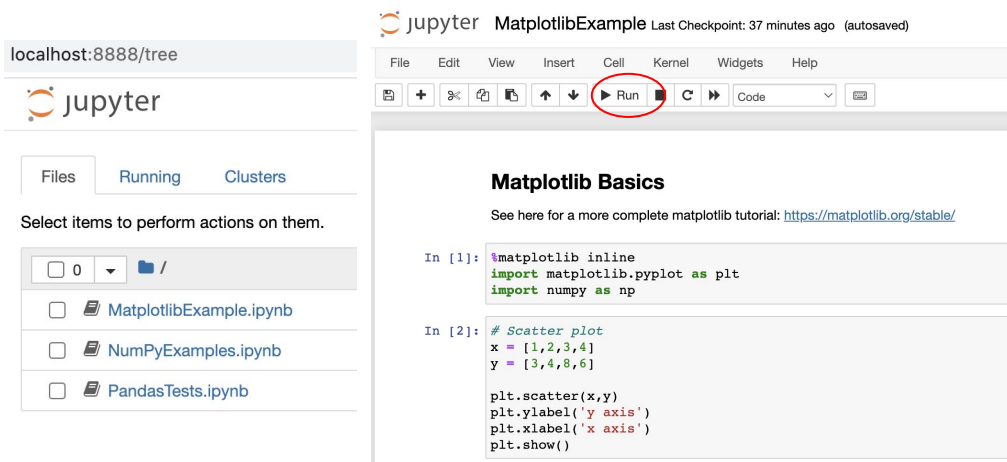
- `pip install <pkg/lib>` (or `pip3` instead of `pip` for python version 3.\*)
- `conda install <pkg/lib>`
- `brew install <pkg/lib>`

Not all packages are available in homebrew or anaconda default locations

- So far I have made the best experience with `pip/pip3`
- Anaconda has the advantage that it allows to install libraries/packages from other sources (browse available sources for packages [here](#))

Jupyter allows to interactively work with python and provides immediate feedback, very useful for tweaking and fine-tuning!

Typing `jupyter notebook` in the terminal will open a browser session including all files and sub-directories of the current directory you are in



localhost:8888/tree

jupyter MatplotlibExample Last Checkpoint: 37 minutes ago (autosaved)

File Edit View Insert Cell Kernel Widgets Help

Run

### Matplotlib Basics

See here for a more complete matplotlib tutorial: <https://matplotlib.org/stable/>

```
In [1]: %matplotlib inline
import matplotlib.pyplot as plt
import numpy as np

In [2]: # Scatter plot
x = [1,2,3,4]
y = [3,4,8,6]

plt.scatter(x,y)
plt.ylabel('y axis')
plt.xlabel('x axis')
plt.show()
```

You can define blocks of code and run through them step by step and separately (attention with inter-block dependencies!)

Once you are done hit “Logout”/“Quit” in the browser or close the program in the terminal where you started the session

Quit

Logout




P.S.: Copy-pasting the code into a \*.py file will give you a python script that you can execute on your machine without jupyter

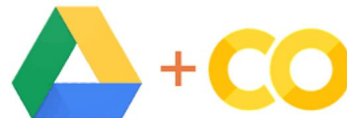
Colab is a Python development environment that runs in the browser using Google Cloud (for free) ; it's also a Jupyter Notebook.

- To download the repo into your Google Drive, use [this Notebook](#)
- Once you ran it (you'll need to give it access to your Drive), just go to My Drive > OxfordCMPP > cmpp and click on any of the Notebooks

My Drive > OxfordCMPP > cmpp > Lecture1\_Introduction ▾



Name	Owner	Last modified	↓	File size
 PandasTests.ipynb	me	9:36 PM	me	18 KB
 NumPyExamples.ipynb	me	9:14 PM	me	5 KB
 MatplotlibExample.ipynb	me	9:14 PM	me	210 KB

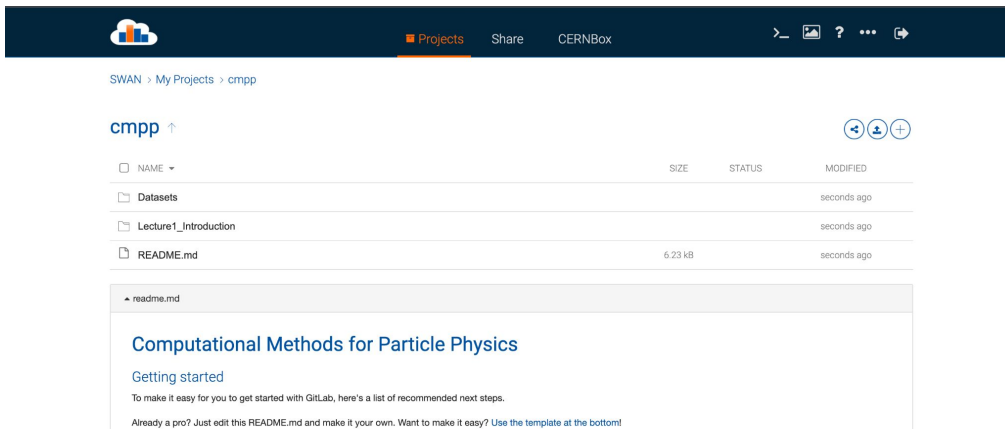


CERN offers a **S**ervice for **W**eb based **A**Nalysis (SWAN): <https://swan.cern.ch>

- Note that you need a CERN account to use it; it can be a lightweight account.



Once your session is started, and you've chosen the configuration (default is OK), you can use the “Download from git” button (see right) and point to <https://gitlab.cern.ch/oxford-physics/cmpp.git>



The screenshot shows the CERN SWAN web interface. At the top, there's a dark blue header with the CERN logo, navigation tabs for 'Projects', 'Share', and 'CERNBox', and a search bar. Below the header, the breadcrumb 'SWAN > My Projects > cmpp' is visible. The main content area shows the 'cmpp' project name with an upward arrow and three icons (left arrow, person, plus). Below this is a table listing project files:

NAME	SIZE	STATUS	MODIFIED
Datasets			seconds ago
Lecture1_Introduction			seconds ago
README.md	6.23 kB		seconds ago

Below the table, the 'README.md' file is expanded, showing the title 'Computational Methods for Particle Physics' and a 'Getting started' section with instructions on how to use the template.



Docker is a system to manage and run containers. A container is a standard unit of software that packages up code and all its dependencies so the application runs quickly and reliably from one computing environment to another.

Very flexible and allows running from any machine with an internet connection and Docker installed; to get Docker, check out <https://docs.docker.com/get-docker/>

```
# Clone the repo
git clone https://gitlab.com/oxford-physics/cmpp.git
# Build the image (once or at every update), from the cmpp folder
docker build -t cmpp docker
# Run the container
docker run --rm -it -p 8888:8888/tcp -v $(pwd):/cmpp cmpp:latest root
--notebook
# Go to http://localhost:8888 and enter the code from the Docker container
```

# Github/Gitlab



Github and gitlab offer free accounts for non-commercial use

You can sign up e.g. via an existing google account or if you have a CERN account it should be connected to CERN's instance of gitlab

For more info, see e.g. this [git tutorial](#)

The diagram illustrates the GitLab project creation and import workflow. It starts with a 'Create new project' section on the left, which includes four options: 'Create blank project', 'Create from template', 'Import project', and 'Run CI/CD for external repository'. Arrows lead from 'Create blank project' and 'Import project' to their respective detailed forms. The 'Import project' form shows options to import from GitLab export, GitLab, or a repository by URL. The 'Create blank project' form shows fields for project name, URL, slug, and description, along with visibility level and project configuration options. Arrows from these forms point to a 'Clone with SSH' and 'Clone with HTTPS' section on the right, which provides the clone URLs and options to open the project in an IDE or clone it.

**Create new project**

- Create blank project**  
Create a blank project to house your files, plan your work, and collaborate on code, among other things.
- Create from template**  
Create a project pre-populated with the necessary files to get you started quickly.
- Import project**  
Migrate your data from an external source like GitHub, Bitbucket, or another instance of GitLab.
- Run CI/CD for external repository**  
Connect your external repository to GitLab CI/CD.

**Import project**

Migrate your data from an external source like GitHub, Bitbucket, or another instance of GitLab.

Import project from  
GitLab export GitLab Repo by URL

**Create blank project**

Create a blank project to house your files, plan your work, and collaborate on code, among other things.

Project name  
My awesome project

Project URL  
https://gitlab.com/eschopf

Project slug  
my-awesome-project

Project description (optional)  
Description format

Visibility Level  
☒ Private  
Project access must be granted explicitly to each user. If this project is part of a group, access will be granted to members of the group.  
☐ Internal  
The project can be accessed by any logged in user except external users.  
☐ Public  
The project can be accessed without any authentication.

Project Configuration  
☒ Initialize repository with a README  
Allows you to immediately clone this project's repository. Skip this if you plan to push up an existing repository.

**Clone with SSH**  
git@gitlab.com:oxford-physics/c

**Clone with HTTPS**  
https://gitlab.com/oxford-physics/c

**Open in your IDE**  
Visual Studio Code (SSH)  
Visual Studio Code (HTTPS)

Find file Web IDE Clone

Gitlab example: creating a new project or import an existing one

Check out the project with  
`git clone <path>`



# User guides for libraries used in today's exercises

---

[Numpy](#)



[Matplotlib](#)



[Pandas](#)

