Python Programming for Chemists: Python Setup

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What you will learn...

- Basics of programming: data structures
- Reading & plotting data with Python
- How to program simple chemical models
- Leverage great tools & libraries from smart people (open source,ChatGPT)
- How to use programming to solve chemical problems!
- Improve your understanding of chemistry by programming!
- **Fun with (Python) programming :-)**

Overview

- **Lectures**
  - Computer & programming basics
  - Python data types & data structures
  - Data analysis & visualization
  - Introduction to scientific computing (numpy&scipy)
  - Outlook: Cheminformatics
- **Assignment**
  - Present a concept for implementing a chemical model / equation
  - Write a small program implementing the model

Useful Textbooks

- Lubanovic, Bill. Introducing Python: Modern Computing in Simple Packages. " O'Reilly Media, Inc.", 2019.
- Hill, Christian. Python for Chemists. Cambridge University Press, 2023.

- Haffner, Ernst Georg. Informatik für Dummies, Das Lehrbuch. John Wiley & Sons, 2023.

Useful Links

Learning Python

https://www.learnpython.org/

https://www.freecodecamp.org/learn/python-for-everybody/

Learning Python via Gamification

https://www.codingame.com/home

https://developer.apple.com/swift-playgrounds/

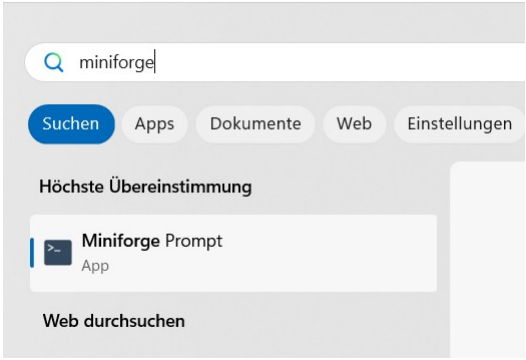
Python Overview / “Cheatsheet”

https://www.utc.fr/~jlaforet/Suppl/python-cheatsheets.pdf

Installation of Python on Windows

- Go to the **miniforge** releases page on GitHub: https://github.com/conda-forge/miniforge#miniforge
- **Download** the installer for Windows (MiniForge-<version>-Windows-x86_64.exe)
  (change browser in case you get problems)
- Locate the downloaded installer and double-click to **run**.
- Follow the prompts to complete the installation. Choose **default installation** options.
- You should now have a "**Miniforge Prompt**."
  Type miniforge in windows search bar to find it:
- **Change directory** to Z: (no write permissin in C:)
  `Z:`
- Create your own **Python environment**:

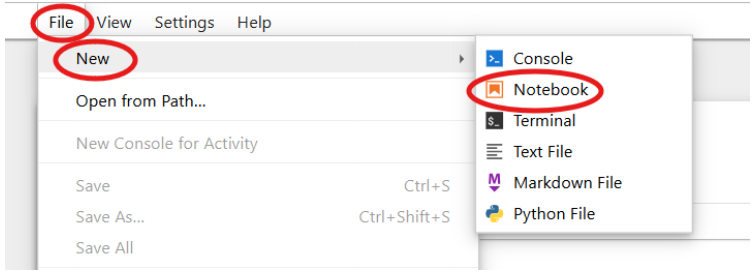
```
mamba create -y -n myenv python=3.11
```



Starting Interactive Python Session

- Activate the environment:
  `mamba activate myenv`
- Install the package `jupyter`:

  `mamba install -y jupyter notebook`
- Start juypter notebook server: `jupyter notebook`
- Go to: `File → New → Notebook`
- Select kernel: `"Python3"`



- Within the notebook cell, type: `print("Hello!")` and press **shift+return**

Jupyter Notebook / Lab

Why Jupyter?

- **Interactivity**
- Prototyping & fast iterations
- Visualization
- Can be used for “computer experiments”
- **Documentation** via Markdown

When not to use:

- Do not use them for large programs and when building libraries → IDE

Jupyter notebooks

- **Cells**
  - Code Cells: interactive programming – run `shift+enter` for code execution
  - Code is executed one cell after another
  - Markdown Cells: documentation & formulaes
- **Kernel**
  - Computational engine: Mostly python, but also other languages possible
  - Restart the kernel to delete all variables
- Special (magic) commands: **%**time or e.g. **!**ls for command line options
- Autocompletion: use `Tab` to get suggestions for functions!
- Widgets: Build simple graphical user interfaces

Integrated Development Environment (IDE)

- Use a IDE for more heavy-weight programming
- An IDE is much more than a text-editor:
- autocompletion, code highlighting, debugging, searching,code navigating, renaming, refactoring, testing ...
- Important IDEs for Python:
  - VSCode: Very general & powerful – most used IDE
  - Pycharm: Customized for Python and data science apps
  - Thonny: Minimalistic – for beginners

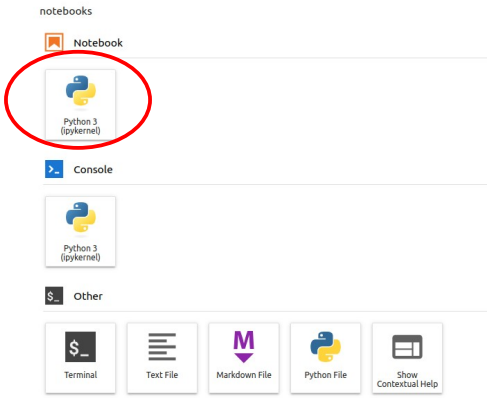
Installation of IDE (thonny)

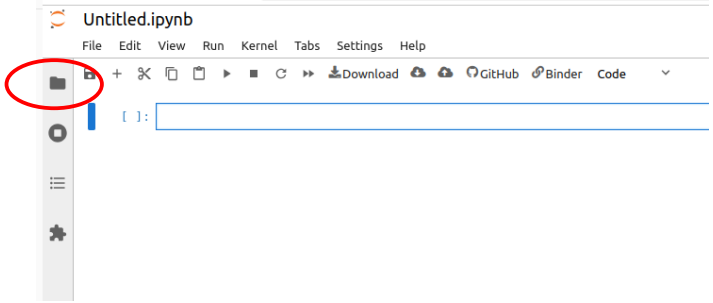
- Go to https://thonny.org/
- Download portable variant python 3.10 64bit
- Extract file in Downloads folder
- Copy directory to Z:
- Start IDE by clicking on thonny.exe

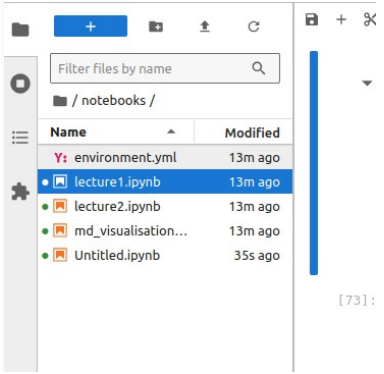
Browser based access

- Use this link in your browser:

  `https://mybinder.org/v2/gh/CHLoschen/ProgrammingForChemists24/main?labpath=notebooks`







Additional Material

Technical links

- Sharing notebooks via binder: https://ovh2.mybinder.org/
- Setup jupyter: Working with **jupyter notebooks** for programming: https://docs.jupyter.org/en/latest/running.html
- setup binder: https://jupyter.org/binder
- setup colab: https://course19.fast.ai/start_colab.html
- Working with **github** for versioning control: https://docs.github.com/en/get-started/start-your-journey/hello-world
- Working with **jupyter notebooks** for programming: https://docs.jupyter.org/en/latest/running.html
- How to open github notebook with colab documention: Open github notebook with colab
- Open Notebook in browser from github or google drive:
- https://colab.research.google.com/github/chrissly31415/lecture_cheminformatics
- Open master branch:https://colab.research.google.com/github/chrissly31415/lecture_cheminformatics/blob/master
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