

Hands on Machine Learning for Fluid Dynamics

7 – 11 February 2022



Lecture 0 **Before we start....**

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...be prepared!

For the course you need:

- a laptop
- a working Python environment (**Python3 only!!!**)
- to install the required packages
- an editor

Please note that we will use the latest version of each package.

Therefore, we strongly recommend you create a new environment from scratch (see instructions in this document)

Install Python on Windows

- Use Anaconda (**strongly recommended**) :
<https://www.anaconda.com/distribution/#download-section>
- Use Windows Sub Linux (**most flexible - linux like**)
(then see Python on Linux slides after installation)
- Install WSL: <https://docs.microsoft.com/en-us/windows/wsl/install-win10>
- Install vcxsrv for graphical rendering: <https://sourceforge.net/projects/vcxsrv/>
- Use Python package (**less integrated with editors f.e.**):
<https://www.python.org/downloads/windows/>

Install Python on Linux

- Through Linux distribution (example for Ubuntu):

```
sudo apt update
```

```
sudo apt install python3 python3-pip
```

```
sudo apt install python3-dev build-essential
```

- Using Anaconda: <https://www.anaconda.com/distribution/#download-section>

Install packages on Windows

- Using the Anaconda interface
- Using the Anaconda prompt (recommended!):

If the package exists in the Anaconda distribution

```
conda install package_to_install
```

If not available in the Anaconda distribution, use pip

```
python -m pip install package to install
```

Install packages on Linux (including WSL)

Run the following on the shell

```
python3 -m pip install package_to_install --user --upgrade
```

where:

--user puts the package in the user's folders (no need of sudo rights)

--upgrade updates the package if needed

Or you can use the same `conda` command as on Windows, if Anaconda is used.

Create an environment in Conda

This step is not necessary but strongly advised.

Environments have specific versions of packages and avoid compatibility issues. This is a good practice: you can have different versions of the same package on different environments. They also allow to install packages without root permissions.

An alternative to conda environments are `virtualenvs`
(see <https://docs.python.org/3/library/venv.html>)

To create an environment for the course called `ML_course` with python 3.8:

```
conda create -n VKI_ML_course python=3.8
```

To activate the environment:

```
conda activate VKI_ML_course
```

Packages we will need in the course

This is the list of packages we will need

- numpy
- scipy
- modulo_vki
- pandas
- matplotlib
- scikit-learn
- imageio
- shutil
- latex
- gym
- scikit-optimize
- deap
- torch
- tensorflow

Please note that for some of these packages the order of installation matters!

Installation Procedure for Anaconda users (1)

For Anaconda users, follow this procedure step by step:

Step 1. Open the Anaconda Terminal (with administration permission). Create an environment for the course and activate it:

```
conda create -n VKI_ML_course python=3.8
```

You can check that this is now available by typing:

```
conda env list
```

Then, you can activate it by typing

```
conda activate VKI_ML_course
```

Installation Procedure for Anaconda users (2)

Step 2. Make sure you have the latest version of pip tools: (press Y when asked)

```
conda install pip
pip install --upgrade pip pip-tools --user
```

Step 3. Install the Spyder editor if needed (see <https://www.spyder-ide.org/>)
(press Y when asked)

```
pip install --upgrade --user PyQtwebengine==5.12.1
pip install --upgrade --user PyQt5==5.12.3
conda install spyder
```

Installation Procedure for Anaconda users (3)

Step 4. Install the following packages first (press Y when asked)

```
pip install modulo_vki latex numpy matplotlib pandas scipy imageio  
pip install pytest-shutil
```

Installation Procedure for Anaconda users (4)

Step 5. Now install the more advanced ones (press Y when asked)

```
pip install tensorflow torch deap scikit-learn gym scikit-optimize
```

Note: if you encounter the following error:

```
modulo-vki 1.1.3 requires numpy==1.19.5, but you have numpy  
1.22.1 which is incompatible.
```

Do not worry about it. The modulo package will still run!

Test your installation before the course

Go in the working directory and run the file 0_TEST_ME.py. You can now open spyder from the terminal (typing 'spyder') or you could just type:

```
python 0_TEST_ME.py
```

All the essential packages should be listed as available. Ignore errors from tensorflow asking for an installed GPU, in case you do not have one.

We will not use the GPU functionalities in this course.

Alternative editors

We strongly recommend using Spyder (Included in Anaconda distribution), especially for beginners. This is the one we will use in the course.

However, if you are really looking for alternatives, good options are:

- pyCharm (<https://www.jetbrains.com>) (common for advanced users)
- Thonny, simplified IDE for beginners (<https://thonny.org>) (minimalistic)
- Visual Studio Code (<https://code.visualstudio.com/>), supports python/WSL as interpreter. This is also common among advanced users.

Useful resources to learn Python

- Some online material NumPy for Matlab users:

<https://numpy.org/doc/stable/user/numpy-for-matlab-users.html>

- Basic course: <https://techwithtim.net/tutorials/python-programming/beginner-python-tutorials/variables-data-types/>

- Basic computing: https://scipy-lectures.org/intro/language/python_language.html

- More advanced: <https://docs.python.org/3/tutorial/>

Suggested books

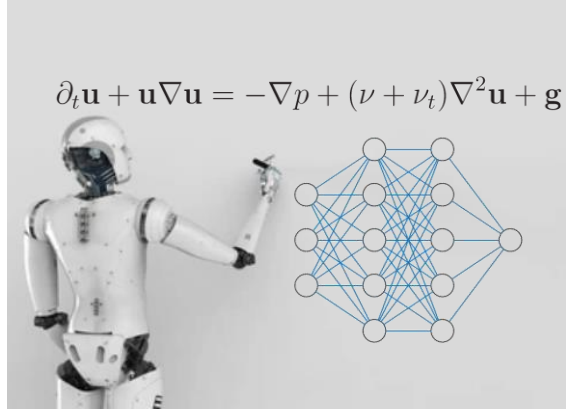
- Python Data Science Handbook by Jake VanderPlas, O'Reilly 2016

(<https://jakevdp.github.io/PythonDataScienceHandbook/>)

- Programming for Computations- Python, S. Linge- H.P. Langtangen, SpringerOpen 2019
- A Primer on Scientific Programming With Python S. Linge- H.P. Langtangen, SpringerOpen 2009

- Numpy and Scipy, by Eli Bressert, O'Reilly 2012

- Foundations of Applied Mathematics Series by Jeffrey Humpherys, T. J. Jarvis, E. J. Evans (<https://foundations-of-applied-mathematics.github.io/>)



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Looking forward to meeting you!

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