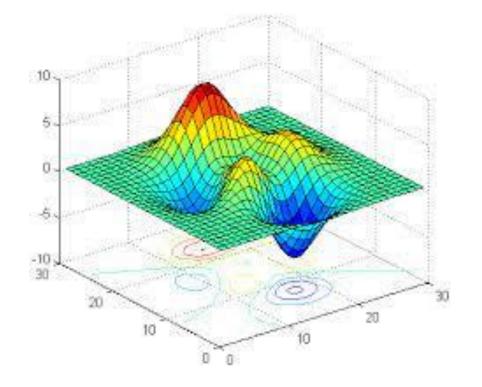


### **Khemis Miliana University**

Faculty of Sciences of Matter and Computer Science Department of Physics





# Numerical Methods & Scientific Programming

Dr. Salah-Eddine BENTRIDI

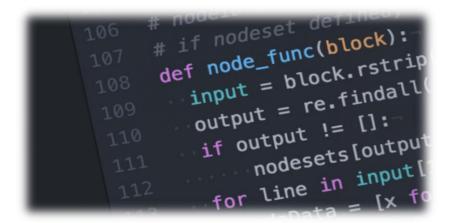
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Univ. Khemis-Miliana

## Content of the program

- Chapter 01: Initiation to a programming language (Python)
  - Hands-on-Pythn; Basics of Python
- Chapter 02: Numerical Integration
  - Trapezoidal rule; Simpson's method
- Chapter 03: Numerical Solution of equations
  - Bisection method; Newton's Method
- Chapter 04: Numerical resolution of differential equations
  - Euler's method; Runge-Kutta method
- Chapter 05: Numerical resolution of linear equations system
  - Gauss method, Gauss-Seidel method









# **Hands-on Python**

An open-source programming language



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Chapter 01: Initiation to a programming language

## **Outline**

- What is Python?
- Why Python?
- How to work with Python?
- Getting started with Python: Installation and first steps
- The basics of Python
- Python for computational and numerical physics



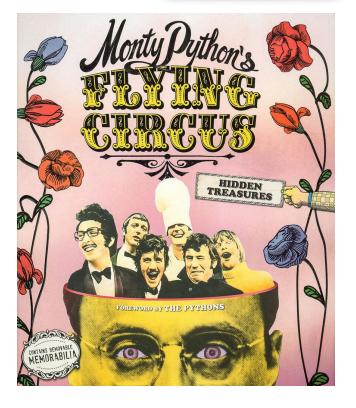




- Python is a general-purpose, high-level, interpreted language known for its ease of use, extensive libraries and tools, and code readability;
- Created and developed by Guido VAN ROSSUM (NL) since 80's. First release was in 1991 (Python0.90);
- It was designed to work initially only on linux-like platform, but fortunately since 2019 it could be supported by Windows (8, 10, 11);
- The name Python comes from an old BBC television comedy sketch series called Monty Python's Flying Circus.







## What is Python?

#### The Zen of Python: Guiding principles for writing computer programs

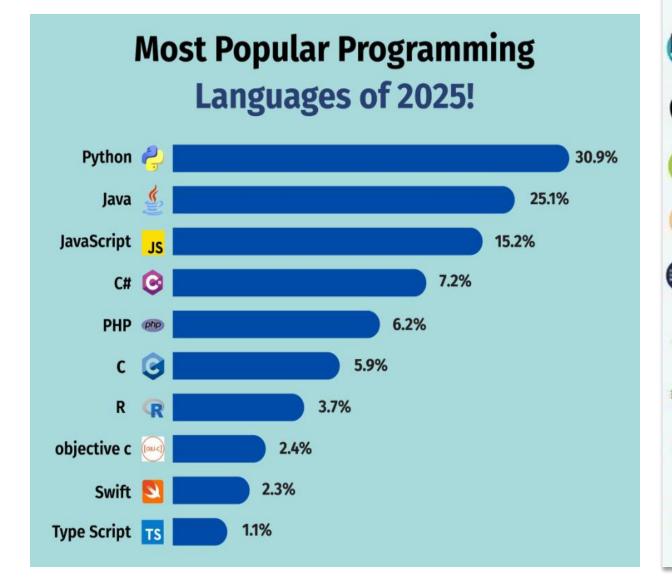
- Beautiful is better than ugly.
- Explicit is better than implicit.
- Simple is better than complex.
- Complex is better than complicated.
- Flat is better than nested.
- Sparse is better than dense.
- Readability counts.
- Special cases aren't special enough to break the rules.
- Although practicality beats purity.
- Errors should never pass silently.

- Unless explicitly silenced.
- In the face of ambiguity, refuse the temptation to guess.
- There should be one-- and preferably only one --obvious way to do it.
- Although that way may not be obvious at first unless you're Dutch.
- Now is better than never.
- Although never is often better than right now.
- If the implementation is hard to explain, it's a bad idea.
- If the implementation is easy to explain, it may be a good idea.
- Namespaces are one honking great idea let's do more of those!

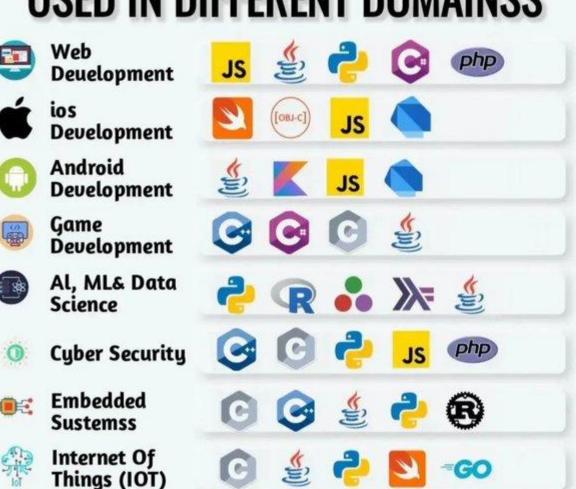
## Why Python?

- It is easy to learn: shorter time is required than many other languages;
- It is easy to use for writing new software : codes could be written faster with Python;
- It is easy to obtain, install and deploy: it is free, open and multiplatform;
- Python can handle complex algorithms and is excellent for data automation, making it a natural fit for Machine Learning (ML).
- Being open-source, it has support from a large community of Python users committed to making it better and more efficient.

## Why Python?



# PROGRAMMING LANGUAGES USED IN DIFFERENT DOMAINSS



Blockchain Technology

The terminal (interpreting line by line)

```
a = 1
b = 2
c = a + b
print('a + b is', c)
```

```
Select Command Prompt
C:\Users\saber>_
```

• The interactive terminal  $\mathbf{TP}[y]$ :

```
q1_spending = 50

q2_spending = 60

total_spending = q1_spending + q2_spending
print('total spending is ', total_spending)
```

```
(base) saber@saber-X1:~$
```

Text editor



```
File Edit View Selection Find Packages Help

my_code.py

1    a = 1
2    b = 2
3    c = a + b
4    print('a + b is ', c)
5
```

```
Command Prompt
C:\Users\saber\Documents>
```

# How to work

## with Python?

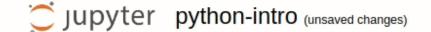
Integrated

**Development** 

**Environment** 

(IDE): Jupyter







Not Trusted

Logout

Python 3 O



#### 6. Using Modules to Load Data

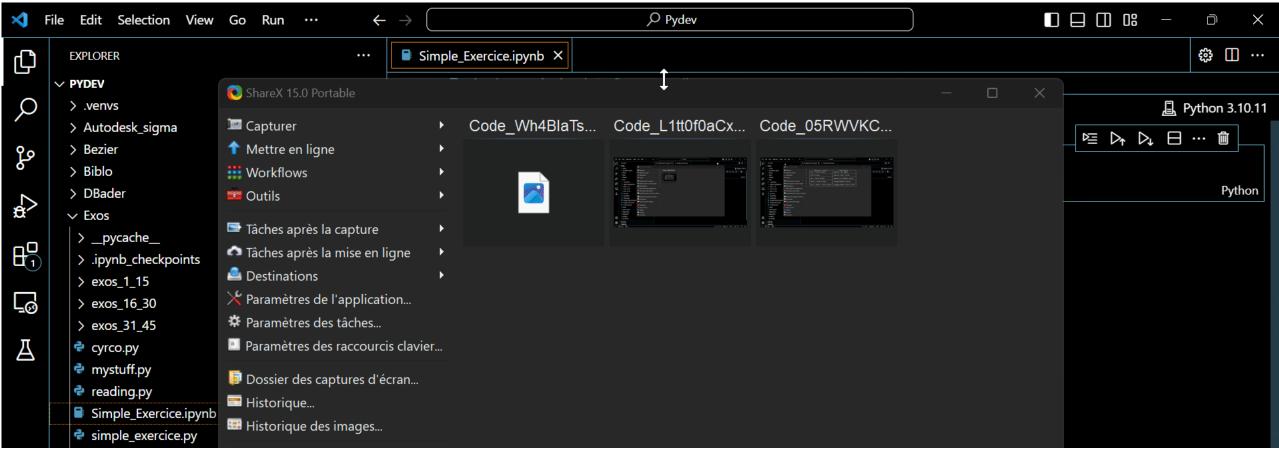
Can we use a module to load the data into python and avoid all the code we used earlier? The answer is YES! We can use pandas. Pandas is like having MS EXCEL in python, but just more powerful. Here is an example.

#### 7. Plotting Data Loaded Using pandas

Plotting this data is very simple. Just pick which columns to plot.

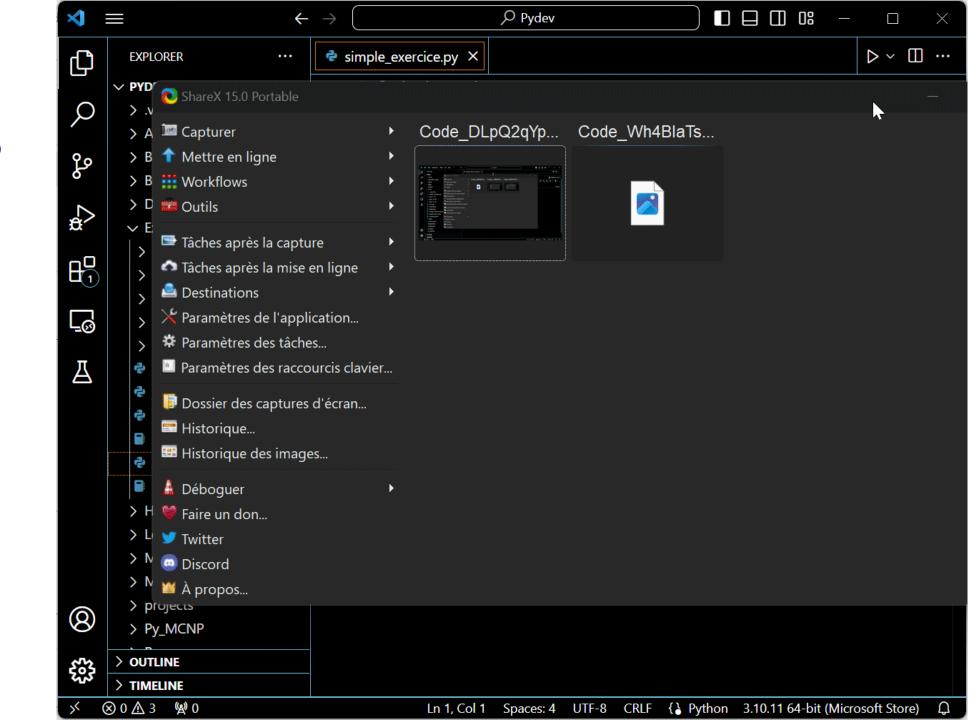
• Integrated Development Environment (IDE): Vscode





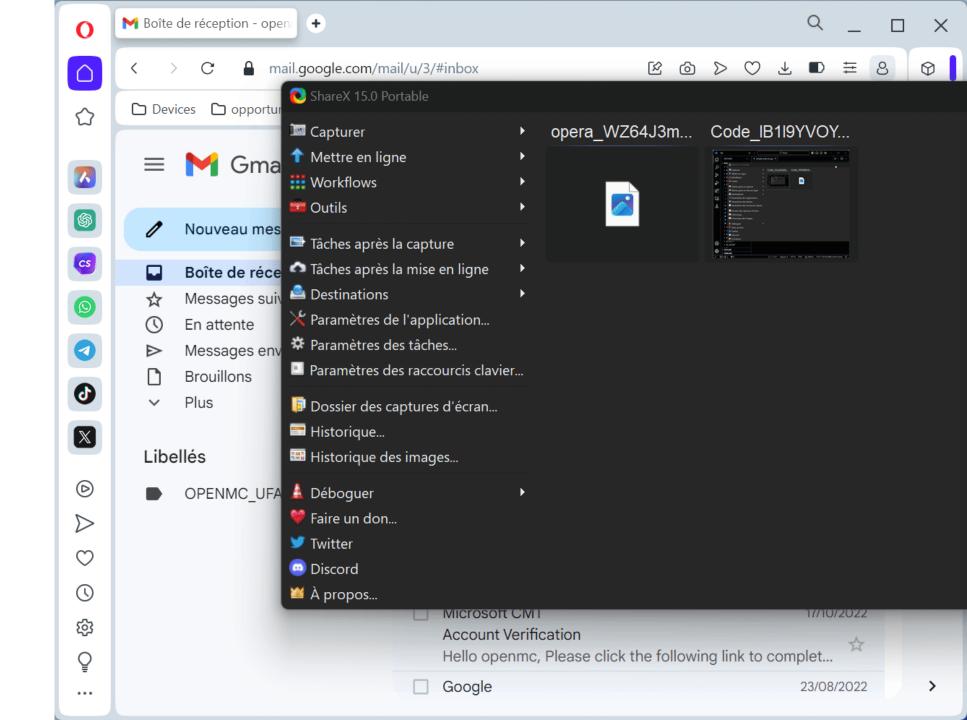
IntegratedDevelopmentEnvironment(IDE): Vscode





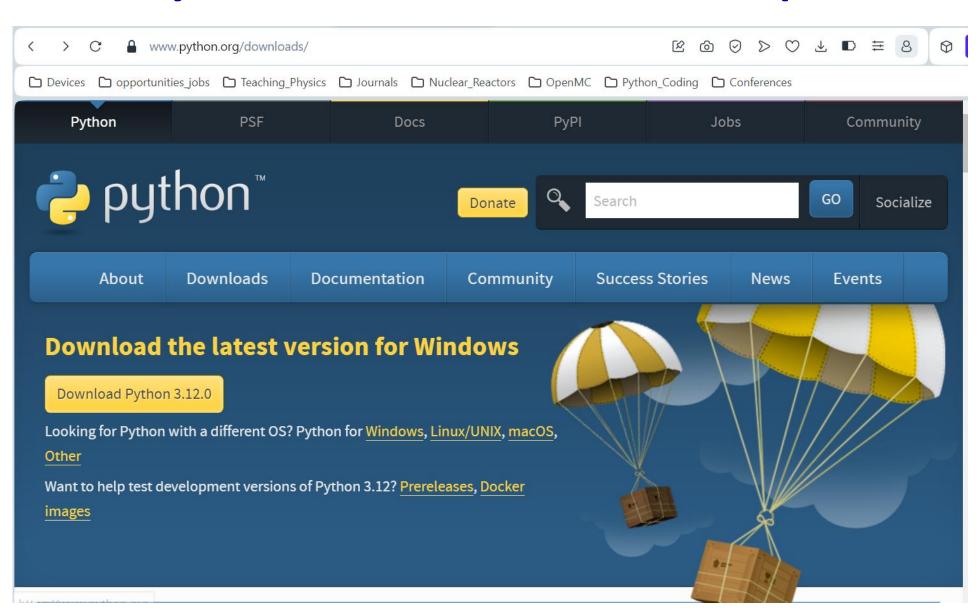
Development
Environment
(IDE): googlecolab





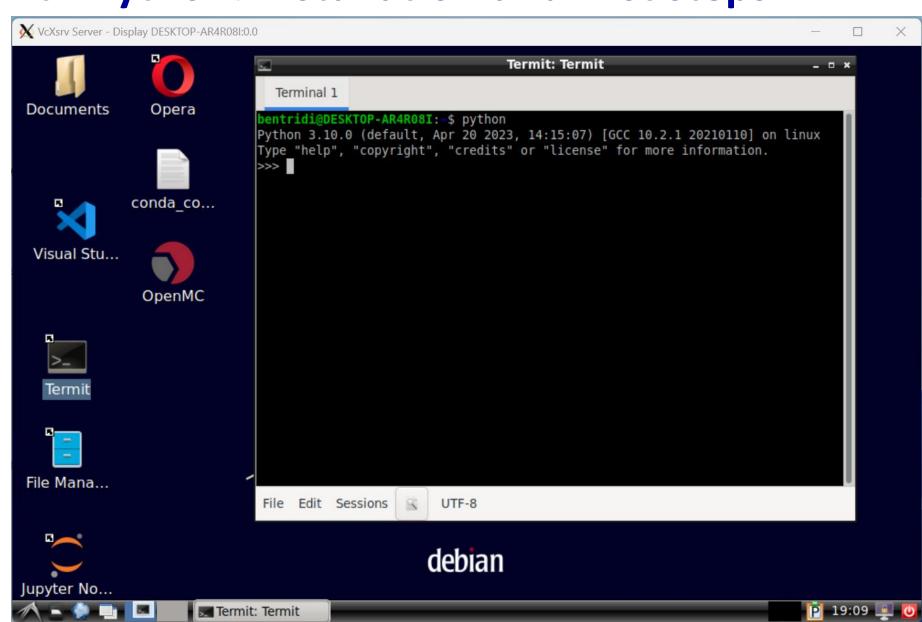
#### For windows users:

Download the installer the given release of Python

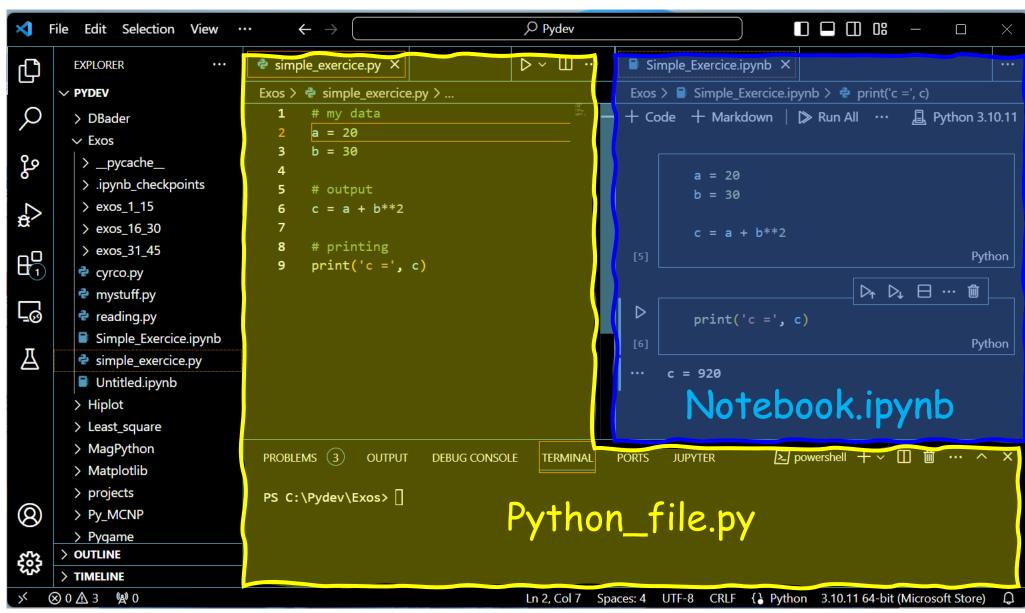


#### For Linux users:

 The Python is already available with the most used Linux distribution: Ubuntu, Debian, Suse, ...



Once vou have **Python** on your machine, is recommended to choose the suitable editor for coding programming and **(VSCODE** or any similar IDE other editors)



is lt also Exercice001.ipynb Commentaire Partager Toutes les Fichier Modifier Affichage Insérer Exécution Outils Aide recommended to modifications ont + Code + Texte **Fichiers** Google.colab use B  $\blacksquare$ since no installation A simple exercice ... sample\_data required. You find the sum of two numbers have access directly to a Linux platform with python already Now print the result installed print('c =', c) <> c = 920=: Disgue 81.27 GB disponible(s) ✓ Connecté à Backend Google Compute Engine Python 3 ×

## The basics of Python

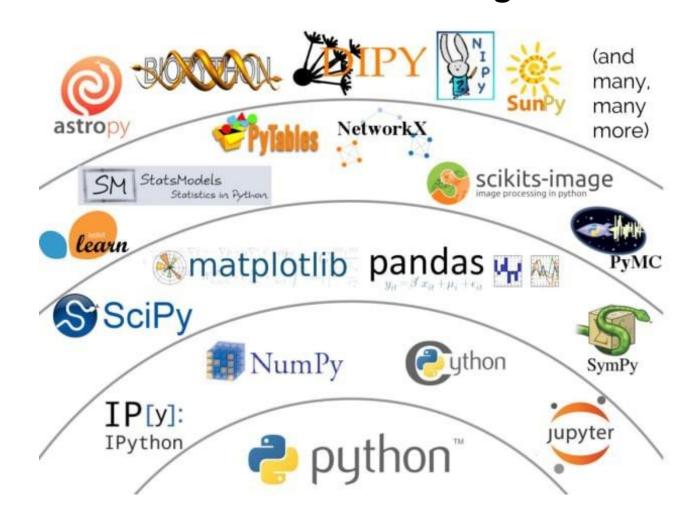
- Some syntax rules
- Variables
- Data types I
- Formatting
- Data types II
- Operators
- User input
- Flow control: if elif else for while
- Functions
- Scope: Local and global variables
- Modules



#### Modules and Libraries: The most used ones for computational physics



#### More than 130.000 existing libraries



#### **PIP: Package Installer for Python**



You need just to type in a command line:

> pip install <package\_name>

for example, to install numpy (numerical python), type:

> pip install numpy