An introduction to Python

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How to get Python (+ useful packages ...)

We are going to use the **miniconda** installer, which is cross-platform and provides package management, together with the **spyder** IDE.

1. Go to https://conda.io/miniconda.html
   (or Google search : "miniconda download")
2. Depending on the operating system, download installer (Python 2.7)
3. Install Python and required packages
   - Mac OS X or Unix:
     3.1 Open a terminal
     3.2 Run "bash Miniconda[...].sh", and yes for all ...
     3.3 Open a new terminal, or run "source ~/.bashrc"
     3.4 Run "**conda install spyder numpy scipy matplotlib sympy**"
   - Windows:
     3.1 Double-click on the .exe file, and yes for all ...
     3.2 Open "conda prompt" terminal (installed with miniconda)
     3.3 Run "**conda install spyder numpy scipy matplotlib sympy**"

What are we talking about

A little history

- Programming language conceived by a Monty Python fan in the 80's
- First released in 1991, then
  - Python 2 in 2000 (community backed development, support $\rightarrow$ 2020)
  - Python 3 in 2008 (major revision)

Current versions (2.7, 3.6) are not entirely compatible, but very close

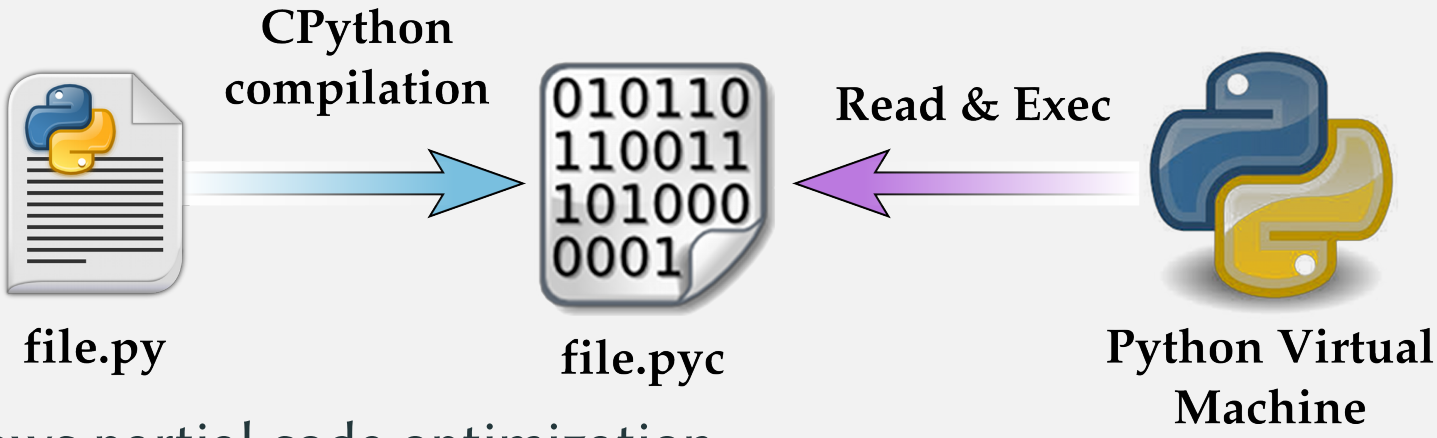
Main motivations

Developers wanted to create a language that would be

- general purpose (they really got that !)
- highly extensible and modular (dynamic language)
- beautiful, simple, **easily readable**

Functioning principles

Pre-compilation of code files



- Allows partial code optimization
- Totally transparent to user
- Portability on every architecture

Python core (Virtual Machine) is written in C:

- Easy interface with other compiled languages (C/C++, Fortran)
- Same speed for read/write files as C

Python vs. Others (Matlab, Fortran, C/C++, ...)

- License-free and open-source ($\neq$ Matlab)
- Huge users community, many (free) packages for many applications
- Extremely easy of use for non-I-love-programming people ($\neq$ Fortran, C/C++)
- Computation can be accelerated using Fortran or C/C++ library ...
- Can scale to very large problems (parallel computing, ...)
- Structured and friendly ways for developing library ($\neq$ Matlab)

Python = many advantages, with very few drawbacks !

Practical tools

Using python console

```
lunet@matlnx13: ~/Recherche/Enseignement/python-math/examples
lunet@matlnx13:examples$ python
Python 3.6.4 |Anaconda, Inc.| (default, Jan 16 2018, 18:10:19)
[GCC 7.2.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

Running a script

```
lunet@matlnx13: ~/Recherche/Enseignement/python-math/examples
lunet@matlnx13:examples$ python helloWorld.py
1 + 1 = 2
   YAILLLLLE !

lunet@matlnx13:examples$
```

All-in-One solution $\Rightarrow$ **Spyder** !

Hello World!

All the examples and python files are available at:
https://gitlab.unige.ch/Thibaut.Lunet/python-math

A first easy step ...

1. Launch Spyder
   - Windows : double click on an icon somewhere ...
   - Mac OS X or Unix : run "spyder" in terminal
2. Discover a wonderful environment #woaaah
3. Go to lower right corner $\rightarrow$ IPython console
   - write "1+1"
   - press enter ...
4. Go to text editor (middle)
   - write "print('hello world')
   - save and run the file ...

Basic variables types and operations

Slide codes at: python-math/examples/code-examples.py

```
# Integer
n = 1
m = 7 % 3  # m = 1

# Float: By default, double precision!
x = 0.5
y = x/7  # y = 0.07142857142857142

# Complex
z = 1+1j
w = z + x + n  # Automatic conversion, w = 2.5 + 1j

# String
s = 'salut'
t = 'toi'
r = s + t  # r = 'saluttoi'

# Boolean
p = True
q = (n != 1)*p + (n == 1)*(x < 10)*(y >= 0)  # q = True = 1
```

Lists

```
# Lists
l = [1, 2, 5, 6]
# Access elements : l[0] = 1, l[2] = 5, l[-1] = 6
# Slice : l[1:3] = [2, 5]

# Nested list
nl = [['vive', 'la'], ['saucisse', 2], 'Toulouse']
# Access sublist element : nl[0] = ['vive', 'la']
# Access final element : nl[0][1] = 'la', nl[1][0] = 'saucisse'

# List comprehension
l1 = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
l2 = [3 * n + 1 for n in l1 if n % 2 == 0]
# l2 = [7, 13, 19, 25, 31]
```

Dictionary

```
# Dictionaries
d = {'first': 1,
     'second': 'two',
     'third': {'A': [3, 4, 5], 'B': True}}
# Access elements : d['first'] = 1, d['second'] = 'two'
#                   d['third'] = {'A': [3, 4, 5], 'B': True}
#                   d['third']['A'] = [3, 4, 5]
#                   d['third']['A'][1] = 4
#                   d['third']['B'] = True
```

Conditional structures

Tabs matter !

```
# If clause
if 1 == 2:
    print('Tocard')
elif 1 == 0:  # Not mandatory
    print('Toujours pas')
else:  # Not mandatory
    print("OK d'accord")

# For loop
for i in range(5):
    print('i = {}'.format(i))

# While loop
i = 0
while i < 10:
    print('TAIHOOO-' + str(i))
    i += 1
    if i == 5:
        break  # Allows to escape from the while loop
```

Function definition

```
def add(a, b=1): # NO NEED to define the type, b has a default value
    return a + b
# add(0.5, 2) = 2.5
# add(1) = 2
# add() -> ERROR


# Possibility of having a variable number of parameters and outputs
def doSomething(x, y, z, p1=1, p3='red'):
    return p1*(x+y), p3+str(z)  # returns a list of two elements

out = doSomething(1, 2, 3)  # out[0] = 3, out[1] = 'red3'
# -- shorter equivalent way
value, flag = doSomething(1, 2, 3)  # value = 3, flag = 'red3'


# General form of a function (cf. function plot of matplotlib)
def myFuncThatDoThings(*args, **kwargs):
    pass
# args is a list, with non keyword argument (ex: a in add)
# kwargs is a dictionnary, with keywords arguments (ex: b=1 in add)
# * and ** are just a notation to 'unpack' list and dictionnary
# keywords arguments ALWAYS at the end (ex: add(b=1, a) -> ERROR)
```

File I/O

```
infile = open("infile.dat", "r")
# Opens the file for reading

for line in infile:
    print(line)
# We can read each line as a string
# If data is numerical, we can convert via float(line)

infile.close()
# Close file to release memory



outfile = open("outfile.dat", "w")
# Opens the file for writing

s = 'Very important secret message'
outfile.write(s + '\n')
# We can write strings, writing '\n' creates a new line
# If data is numerical, we can convert it via str(x)

outfile.close()
# Close file to release memory
```

Numpy and Scipy, what for ?

Loops in python are (REALLY) slow

$\Rightarrow$ do algebraic computation in C (or Fortran)

Numpy : interface for array manipulation

- Data are stored in contiguous memory location
- Operations on arrays are done in C
- Rely on BLAS implementation for algebraic computation

Scipy : companion package for scientific computing

- Many functions for linear algebra, optimization, interpolation, fft...
- Interface with C and Fortran optimized routine
  (LAPACK, FFTW, QUADPACK, ... and many others !)

Numpy basics I

```
import numpy as np
# Import the package

v = np.array([1, 2, 3])
# v is the 1-dimensional vector (1, 2, 3)
# We can access and modify its elements via v[0], v[1], v[2]

v.shape # returns (3,)


A = np.array([[1, 2, 3], [4, 5, 6]])
# A is the 2x3 matrix:
# /1 2 3\
# \4 5 6/
# We can access and modify its elements via A[i, j]

A.shape # returns (2, 3)

B = np.reshape(A, (3,2))
# B is the 3x2 matrix:
# /1 2\
# |3 4|
# \5 6/
```

Numpy basics II

```
# We can slice matrices:
M = np.array([[1,2,3,4], [5,6,7,8], [9,10,11,12]])

M[1:2, 0:2]          # Matrix [5, 6]
M[0:2]               # First two rows
M[:, 1:3]            # Second and third columns
M[-1, :]             # Last line
# INDEX STARTS AT 0 !!!


# We already have some built-in matrices:
np.zeros((3, 3))         # A 3x3 matrix filled with zeros
np.ones((2, 1))          # A 2x1 matrix filled with ones
np.full((2, 2), 27)      # A 2x2 matrix filled with 27
np.eye(2)                # The identity matrix of dim 2


# Useful operations:
C = B.T          # Transpose
A + C            # Elementwise sum
A - C            # Elementwise difference
A * C            # Elementwise product
A / C            # Elementwise division
np.dot(A, B)     # Matrix product
# And lots of other built-in functions!
```

To go further with Numpy and Scipy

Numpy examples :

- Call Fortran routines to accelerate computations
- Easily read and write files with single line coding

... and more in python-math/examples/numpy directory

Scipy examples :

- Data regression using least square minimization
- Eigenvalue computation of the tri-dimensional advection operator

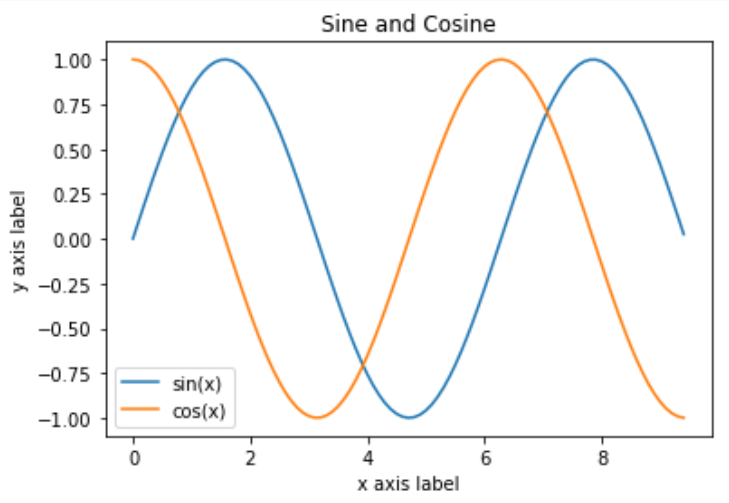
... and more in python-math/examples/scipy directory
See also Scipy tutorials on the Internet

Data visualization with Matplotlib I

```
import numpy as np
import matplotlib.pyplot as plt
# Import the packages

x = np.arange(0, 3 * np.pi, 0.1)
sinx = np.sin(x)
cosx = np.cos(x)
# We generate the data we want to visualize

plt.plot(x, sinx)                    # Draws the points (x, sinx)
plt.plot(x, cosx)                    # Draws the points (x, cosx)
plt.xlabel('x axis label')           # Adds a label to the x-axis
plt.ylabel('y axis label')           # Adds a label to the y-axis
plt.title('Sine and Cosine')         # Adds a title
plt.legend(['sin(x)', 'cos(x)'])     # Adds a legend
plt.show()                           # Actually shows the plot
```

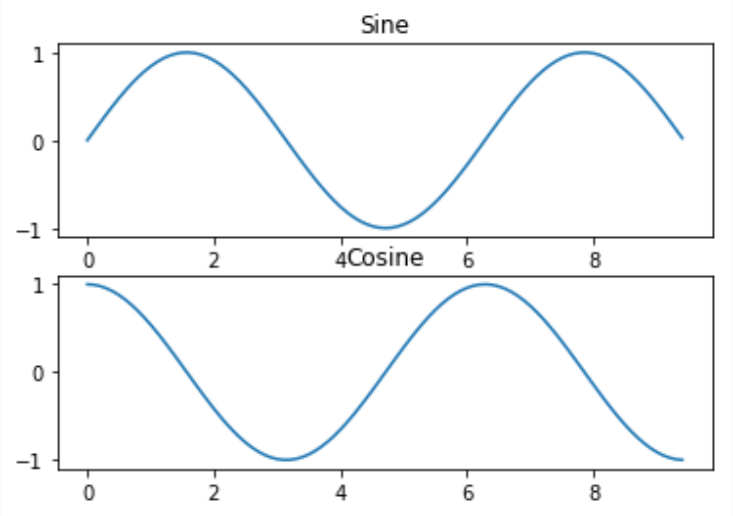


Matplotlib II

```
# We can also display several plots at once:
plt.subplot(2, 1, 1)        # 2x1 grid, select the first as active
plt.plot(x, sinx)
plt.title('Sine')

plt.subplot(2, 1, 2)        # 2x1 grid, select the second as active
plt.plot(x, cosx)
plt.title('Cosine')

plt.show()
```



... and more in python-math/examples/matplotlib directory

Sympy, more than just another py-word game

If you are interested in

- Sparing few neurons by not doing computation by hand
- Verifying some solutions you will give to students
- Obtaining a direct latex translation of some ugly formula

Sympy can help you !

- Symbolic optimized computation core in python
- Can combine numerical calculation with Numpy
- Allow some nice output form within Spyder

To go further with Sympy

Scipy examples :

- Block matrix computation with non-commutative elements
- Compute interpolation formula for non-structured grid
- Latex translation of symbolic formula

... and more in python-math/examples/sympy directory

See also Sympy Tutorials on the Internet

Conclusion

Here was just presented a tiny part of python application for researchers
$\Rightarrow$ many other nice things are also possible

- Writing code documentation, and include math formula
- Create and organize packages for particular applications
- Benefit from the object-oriented programming to facilitate modularity and code development

Do not hesitate to look at python-math/examples for other advanced examples ...

Thanks for watching !
... we hope you enjoy at least some parts ...