

# Scientific python + IPython intro

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#### Headline

- Why python?
- What is python?
- How to use python and IPython?



#### **XFEL** Why Python?



#### The scientist's needs

- Get data (simulation, experiment control, data files)
- Manipulate and process data.
- Visualize results... to understand what we are doing!
- Communicate results: produce figures for reports or publications, write presentations.

#### **XFEL** Existing solutions

- Compiled languages: C, C++, Fortran, etc.
- Scripting languages: Matlab
- Other scripting languages: Scilab, Octave, Igor, R, IDL, etc.



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- General characteristics of Python:
  - clean and simple language: Easy-to-read and intuitive code, easy-to-learn minimalistic syntax, maintainability scales well with size of projects.
  - expressive language: Fewer lines of code, fewer bugs, easier to maintain.
- Technical details:
  - dynamically typed: No need to define the type of variables, function arguments or return types.
  - automatic memory management: No need to explicitly allocate and deallocate memory for variables and data arrays. No memory leak bugs.
  - interpreted: No need to compile the code. The Python interpreter reads and executes the python code directly.

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- Advantages:
  - Very rich scientific computing libraries (a bit less than Matlab, though)
  - Well thought out language, allowing to write very readable and well structured code: we "code what we think".
  - Many libraries for other tasks than scientific computing (web server management, serial port access, etc.)
  - Free and open-source software, widely spread, with a vibrant community.
- Drawbacks:
  - less pleasant development environment than, for example, Matlab. (More geek-oriented).
  - → Not all the algorithms that can be found in more specialized software or toolboxes.

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SciPy (pronounced "Sigh Pie") is a Python-based ecosystem of open-source software for mathematics, science, and engineering. In particular, these are some of the core packages:



NumPy Base Ndimensional array package



SciPy library **Fundamental** library for scientific computing



Matplotlib Comprehensive 2D Plotting

IP[y]: IPython

**IPython** Enhanced Interactive Console



Sympy Symbolic mathematics



pandas Data structures & analysis

#### XFEL Versions of python

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- There are currently two versions of python:
  - Python 2 and Python 3.
  - Python 3 will eventually supercede Python 2, but it is not backward-compatible with Python 2.
  - A lot of existing python code and packages has been written for Python 2, and it is still the most widespread version.
- To see which version of Python you have, run
  - \$ python --version

Several versions of Python can be installed in parallel

### **XFEL** Python interpreter

- For example, to run a file my-program.py that contains python code from the command prompt, use:
  - \$ python my-program.py
  - or run interpretator \$python



### XFEL Why IPython?



- In scientific computing, we typically don't know what we're doing
- IPython is an Interactive shell that addresses the limitation of the standard python interpreter, and it is a work-horse for scientific use of python.
- It provides an interactive prompt to the python interpreter with a greatly improved user-friendliness.



See



#### FEL Ipython, numpy and scipy demonstration

- <u>http://bit.ly/WPG-wiki</u> -> Tutorial files -> Ipython presentation
- Download it
- Run in this folder
  - ipython notebook

### **XFEL** Publishing lpython notebooks

- Generate html and pdf reports
- Free online publishing service <u>http://nbviewer.ipython.org/</u>



## <sup>European</sup>

- Python http://www.python.org/
- Numpy + Scipy + matplotlib <u>http://www.scipy.org/</u>
- H5py <u>http://www.h5py.org/</u>
- Numpy for Matlab users <u>http://wiki.scipy.org/NumPy\_for\_Matlab\_Users</u>
- Free tutorials (some materials was taken in this tutorials)
  - http://scipy-lectures.github.io/
  - http://jrjohansson.github.io/
- Free binary distribution with a lots of scientific stuff (especially for windows users)
  - https://store.continuum.io/cshop/anaconda/
- Free scientific python IDE (Matlab like)
  - https://code.google.com/p/spyderlib/