

# Scientific Python introduction

Iñigo Aldazabal Mensa<sup>\*</sup> <sup>1</sup> Oier Etzaniz<sup>2</sup>

<sup>1</sup> Centro de Física de Materiales (CSIC-UPV/EHU)

<sup>2</sup> UPV/EHU, ACPySS and EuroPythoSociety

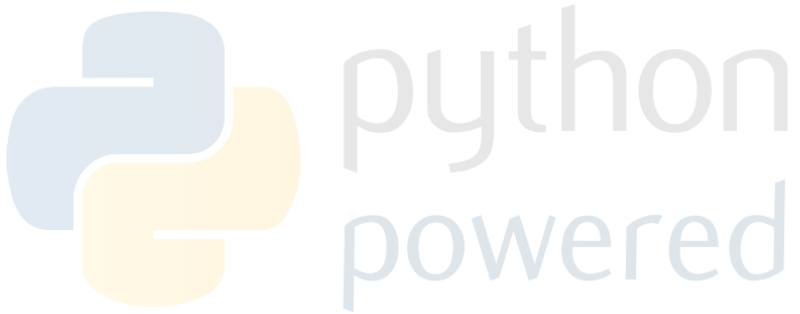
PySS'15 San Sebastián, 23-25th October 2015



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<sup>\*</sup> inigo\_aldezabal@ehu.eus

# Why Python?



```
print("Hello, world!")
```

# Why Python?

Python is inherently slow compared to C/C++ or FORTRAN, so why Python for Scientific Computing?

Python is slow, but...

*Syntactically, Python code looks like executable pseudo code. Program development using Python is 5-10 times faster than using C/C++...*

*The best approach is often to write only the performance-critical parts of the application in C++ or Java, and use Python for all higher-level control and customization.*

*– Guido van Rossum*

# Why Python?

## We have (for free)

- A general purpose language with a huge spectrum of freely available libraries for almost anything you can think of.
- A very easy to learn (and read) language that smoothly interfaces with C/C++ and FORTRAN (eg. calculation kernels).
- Lots of wrappers for well established, fast and long time tested numerical packages.
- Lots of high level utility libraries for scientific computing: plotting, data analysis, parallelization, ...

# Why Python? Batteries Included

## computing in SCIENCE & ENGINEERING

May/June 2007

Computing in Science & Engineering is a peer-reviewed, joint publication of the IEEE Computer Society and the American Institute of Physics



## PYTHON: BATTERIES INCLUDED

# Python Scientific Computing Environment



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  
N-dimensional  
array package



SciPy library  
Fundamental  
library for scientific  
computing



Matplotlib  
Comprehensive 2D  
Plotting



IPython  
Enhanced  
Interactive Console



Sympy  
Symbolic  
mathematics



pandas  
Data structures &  
analysis

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# NumPy



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NumPy is the fundamental package for scientific computing with Python. It contains among other things:

- a powerful N-dimensional array object
- sophisticated (broadcasting) functions
- tools for integrating C/C++ and Fortran code
- useful linear algebra, Fourier transform, and random number capabilities



# NumPy



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```
import numpy as np

# Create a numpy array, a
x = np.array( [1.1, 1.3, 1.5] )
y = np.sin(a)

# create a random two dimensional numpy array, A
A = np.random.rand(3,3)

A.transpose()
A.trace()
```

# SciPy



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SciPy is a collection of mathematical algorithms and convenience functions built on the Numpy extension of Python.

Provides the user with high-level commands and classes for manipulating and visualizing data.

With SciPy an interactive Python session becomes a data-processing and system-prototyping environment rivaling systems such as MATLAB, IDL, Octave, R-Lab, and SciLab.

# SciPy



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## SciPy subpackages (some of them)

- constants: Physical and mathematical constants
- fftpack: Fast Fourier Transform routines
- integrate: Integration and ordinary differential equation solvers
- interpolate: Interpolation and smoothing splines
- linalg: Linear algebra
- optimize: Optimization and root-finding
- signal: Signal processing
- special: Special functions
- ...

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```
import numpy as np
from scipy.special import gamma

x = np.array( [1.1, 2., 3.] )
y = gamma(x)

print (y)
```

```
[ 0.95135077,  1. ,  2. ]
```

# matplotlib



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matplotlib is a python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms.

matplotlib can be used in python scripts, the python and ipython shell (ala MATLAB® or Mathematica®), web application servers, and six graphical user interface toolkits.

For simple plotting the `pyplot` interface provides a MATLAB-like interface, particularly when combined with `IPython`.

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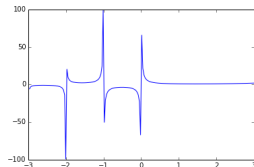


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```
import numpy as np
from scipy.special import gamma
import matplotlib.pyplot as plt

x = np.linspace( start=-3., stop
                 =3., num=200 )
y = gamma(x)

plt.plot(x,y)
plt.savefig("gamma.png")
```



# SciPy



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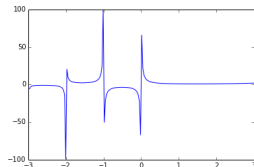


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```



Just google matplotlib images for examples!

# IPython



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IP[y]:  
IPython

IPython  
Enhanced  
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The **IPython Notebook** is a web-based interactive computing system that enables users to author documents that include live code, narrative text, LaTeX equations, HTML, images and video.

These documents contain a full record of a computation and its results and can be shared on email, Dropbox, version control systems (like git/GitHub) or [nbviewer.ipython.org](http://nbviewer.ipython.org).



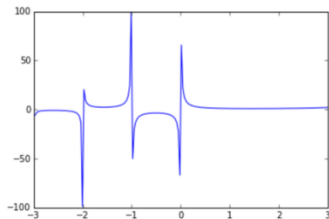
# IPython

```
In [45]: %matplotlib inline
import numpy as np
from scipy.special import gamma
import matplotlib.pyplot as plt

x = np.linspace( start=-3., stop=3., num=200 )
y = gamma(x)

plt.plot(x,y)
```

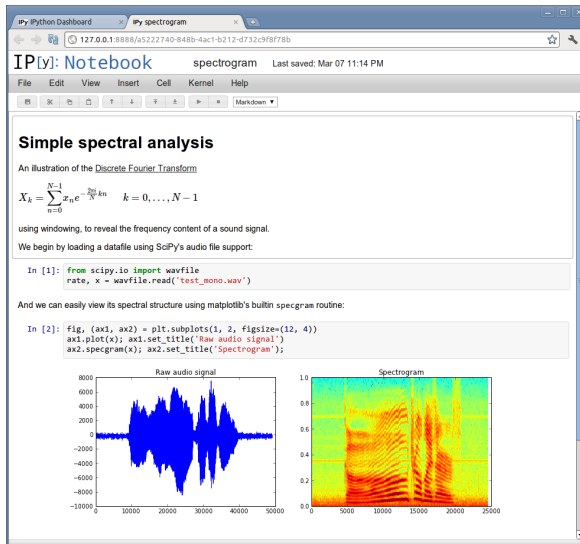
Out[45]: [<matplotlib.lines.Line2D at 0x7fc4ac4660b8>]



In [ ]: |

IP[y]: IPython  
Interactive Computing

# IPython



# Python Scientific Computing Environment



IP[y]:  
IPython

Let's try it!