Get started with scientific Python

Potsdam (February 7-9, 2018)

Benoît Bovy - GFZ, section 5.5

Small survey

First, let's have a look at the results of the survey...

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This may be also challenging for new users.

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- Isn't Python too slow?

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Session 1: introduction to Python

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Session 3: mini-projects

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Session 6: Maintain, share and publish your code

- Good practices of programming and software development

A brief presentation of

The origin of Python

source: wikipedia

Python is not new at all, it was created more than 25 years ago by Guido van Rossum.

Python (CPython) is a community-based, open-source project managed by the Python Software Foundation.

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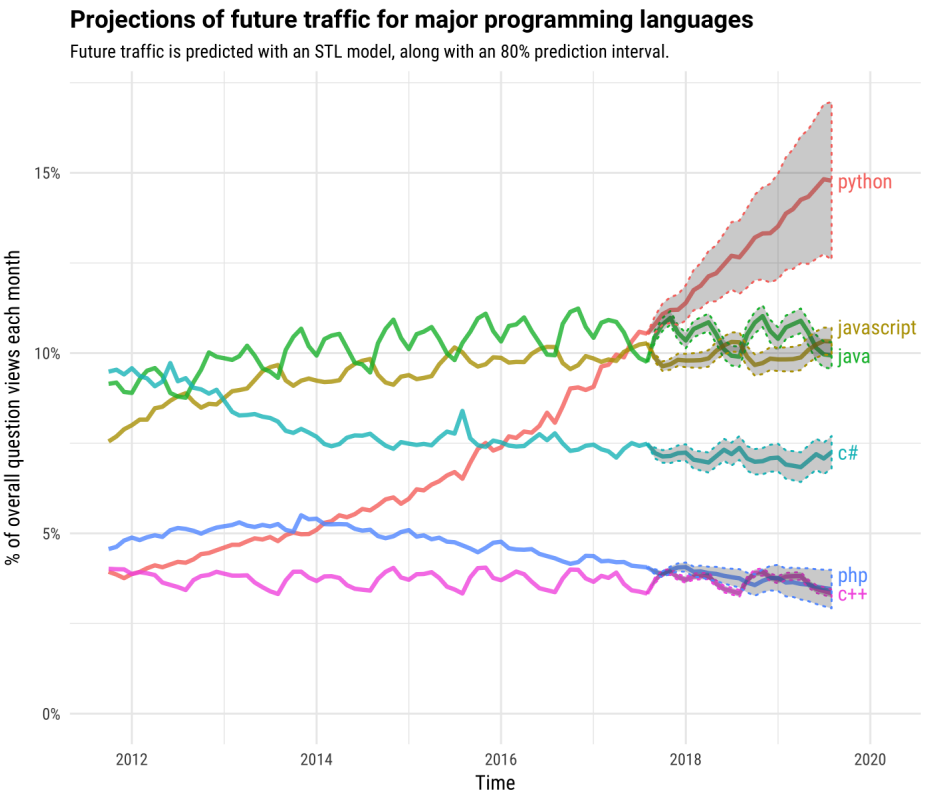
Therefore, hereafter we use "Python" to refer to both the language and the CPython implementation.

The rise of Python

Python has slowly gained popularity over the years with a recent high increase, especially within the scientific community.



source: stackoverflow

Why is Python popular?

Scientific work involves a whole range of different computational tasks.

Numerics

Data management

Text processing

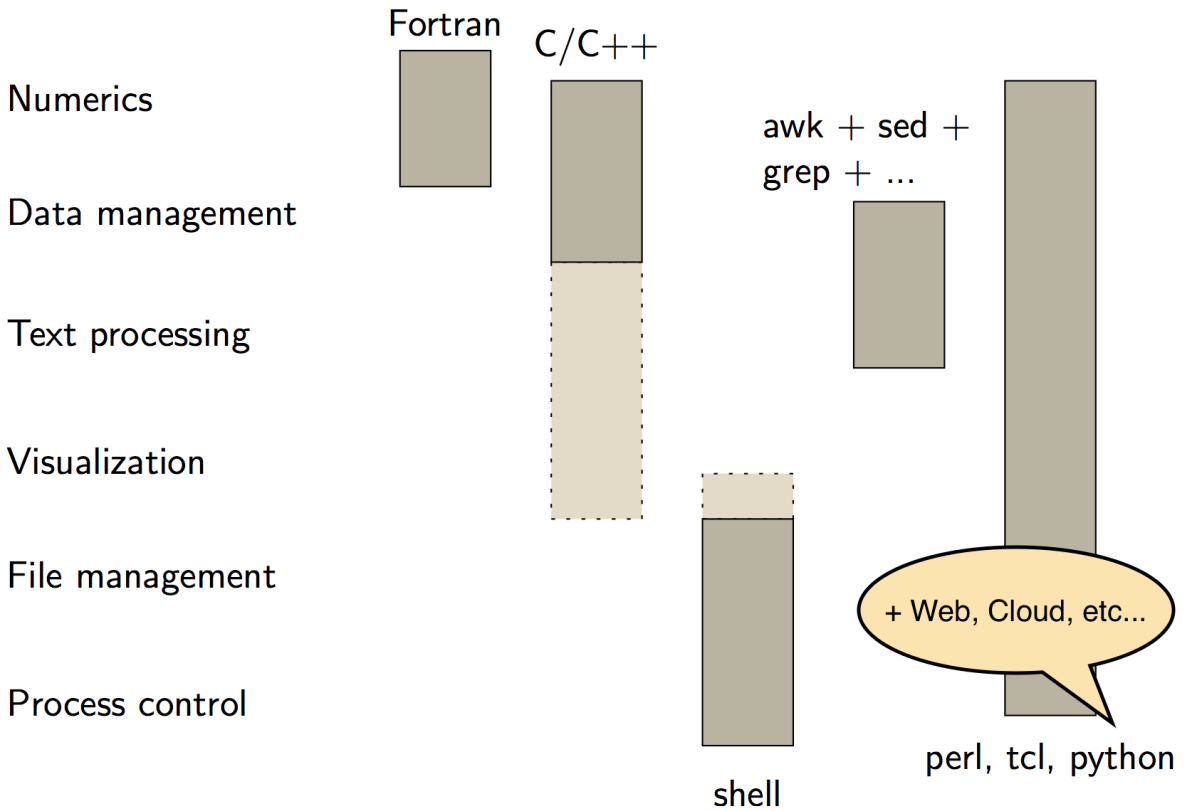
Visualization

File management

Process control

Why is Python popular?

Python is a general purpose language.



source: kinherd.org (Sebastian Heimann)

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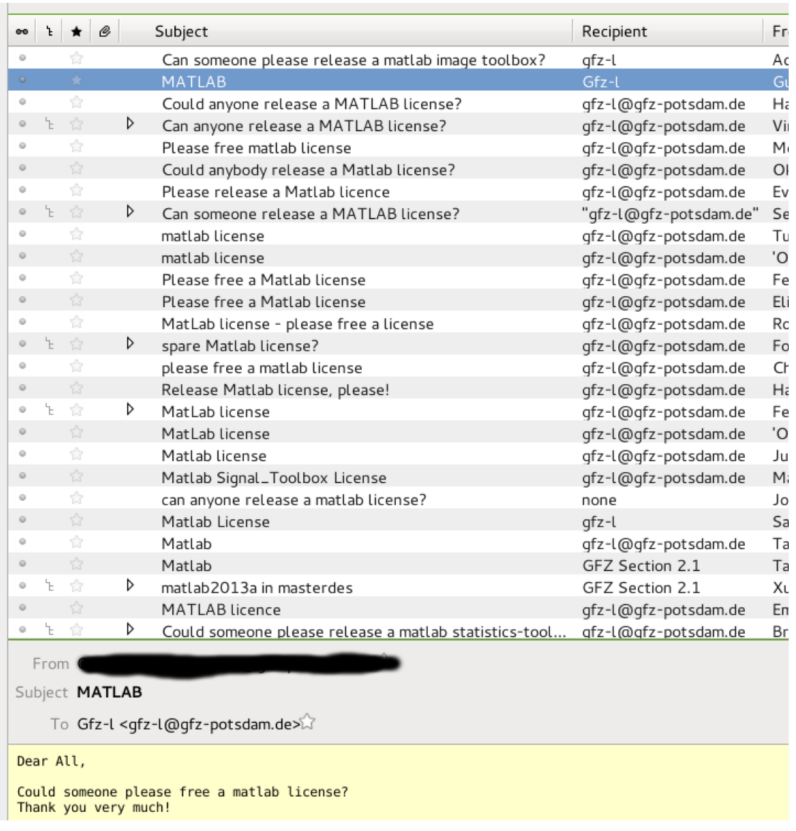

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Can someone please release a matlab image toolbox?	gfz-l	Ac
MATLAB	Gfz-l	Gu
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MATLAB licence	gfz-l@gfz-potsdam.de	En
Could someone please release a matlab statistics-tool...	gfz-l@gfz-potsdam.de	Br

From [redacted]
Subject **MATLAB**
To Gfz-l <gfz-l@gfz-potsdam.de>

```
Dear All,

Could someone please free a matlab license?
Thank you very much!
```

This doesn't happen with Python.

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Multi-paradigm (imperative, object-oriented, functional)

- **Suited for writing small scripts as well as large applications**

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The ecosystem is rapidly and constantly evolving

- Continuous maintenance work

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There are many ways to install Python (CPython) + libraries 🤔

- Plateform-specific package managers (apt, homebrew)
- Cross-platform package managers (conda, pip)
- Python distributions (Enthought, PythonXY)
- Compiling the sources (...really?)

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My advice 😉

- use conda!
- (and pip when a package cannot be installed using conda)

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- A lot of packages available for scientific development
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Useful ressources:

- Conda documentation (including tutorials)
- For geeks: read this blog post

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- Python interactive console

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$ python
Python 3.5.2 |Continuum Analytics, Inc.| (default, Jul  2 2016, 17:52:12)
[GCC 4.2.1 Compatible Apple LLVM 4.2 (clang-425.0.28)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
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- Execute Python scripts (files with *.py* extension)

```
$ python myscript.py
```

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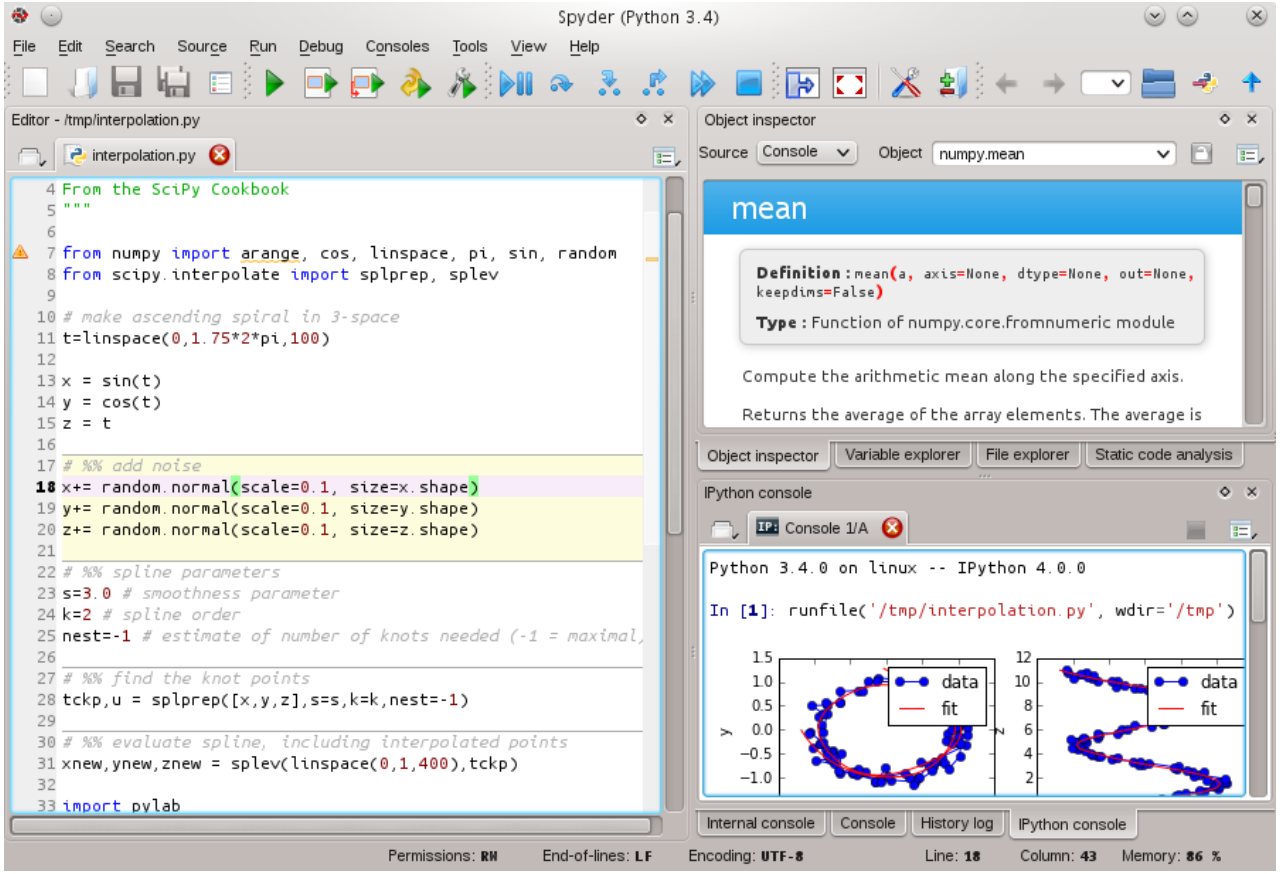
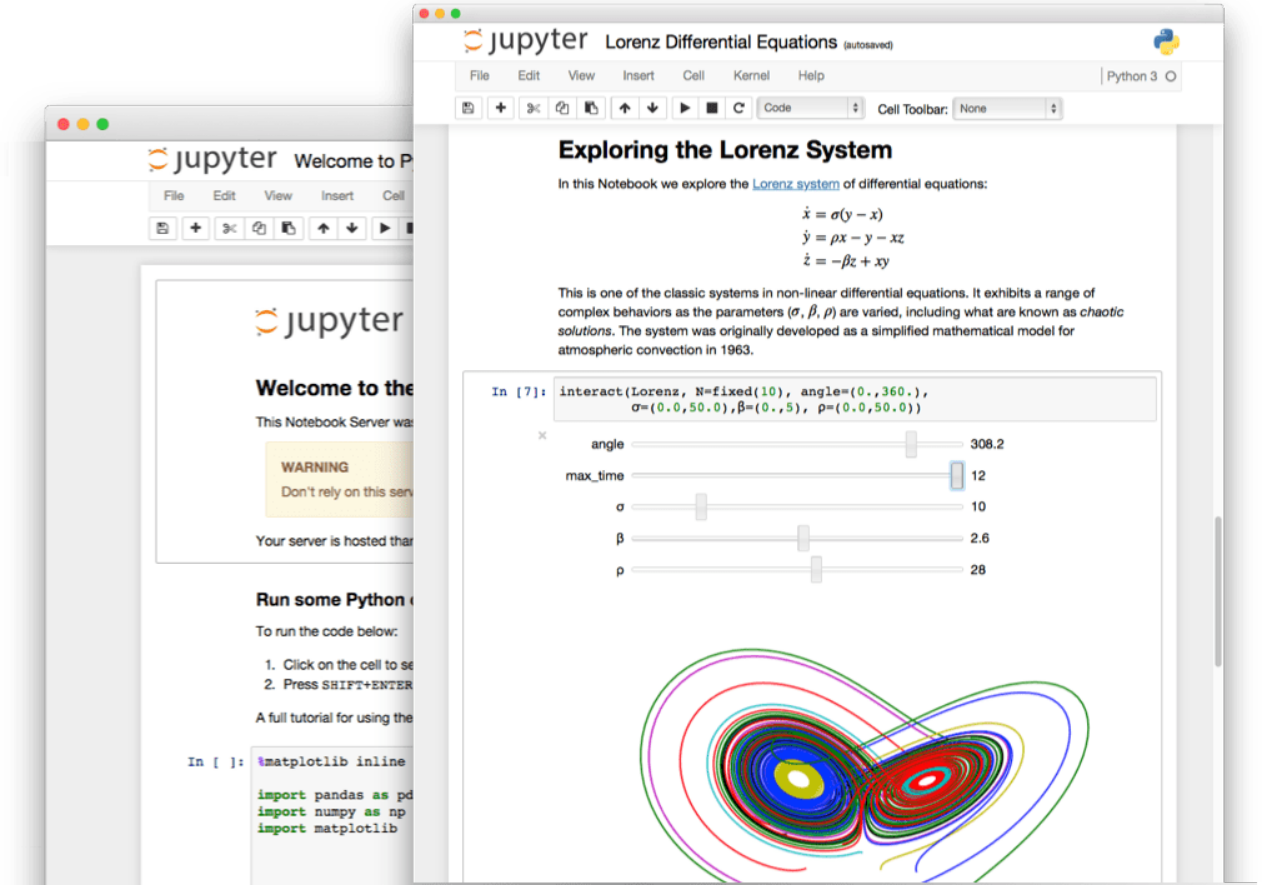
- Spyder (similar to Matlab)



How to execute Python code?

- Jupyter Notebook

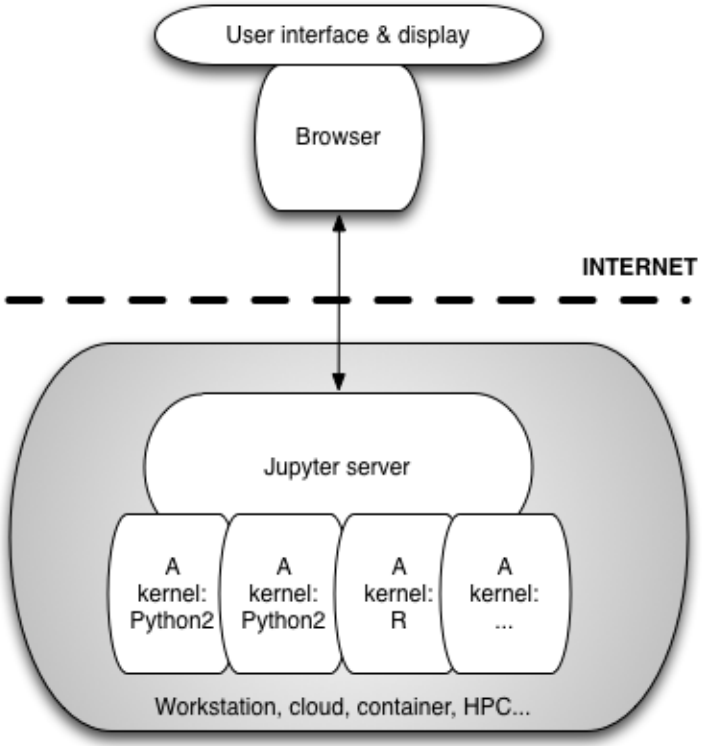


How Jupyter works?

It decouple the interface and the code exectution

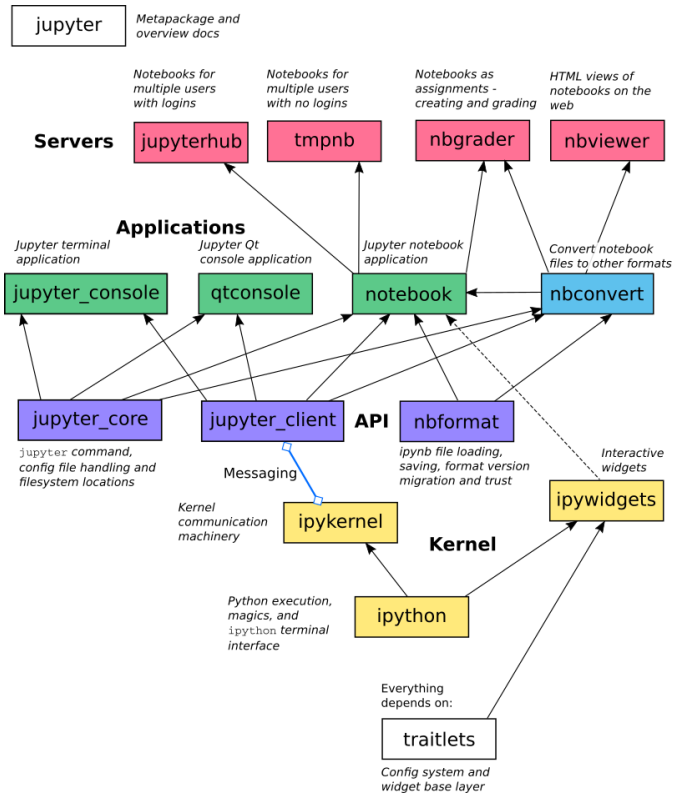
Code can be executed remotely!

Initially for Python (IPython), but language agnostic (R, Julia, Octave... even C++ or Fortran)



source: Oslo repeatability

The Jupyter project: beyond the notebook



source: Jupyter documentation