ESCAPE

European Science Cluster of Astronomy & Particle physics ESFRI research Infrastructures

Python and Notebooks

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Overview

- Introduction
- Python
- Jupyter Notebooks
  - Basic usage
  - Useful features for presenting results
    - How to hide code
    - Jupyter-widgets
    - Slides with Jupyter
- Jupyter Lab
- Binder

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Introduction

- Python
  - Multi purpose, object oriented programming language.
    - Released in 1991 – Guido Van Rossum;
    - Python 1.0 released in 1994.
    - Python 2 was released in 2000 and Python 3 in 2008.
      - Python2.7
      - Python3.9
- Currently one of the most used programming languages.

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Python

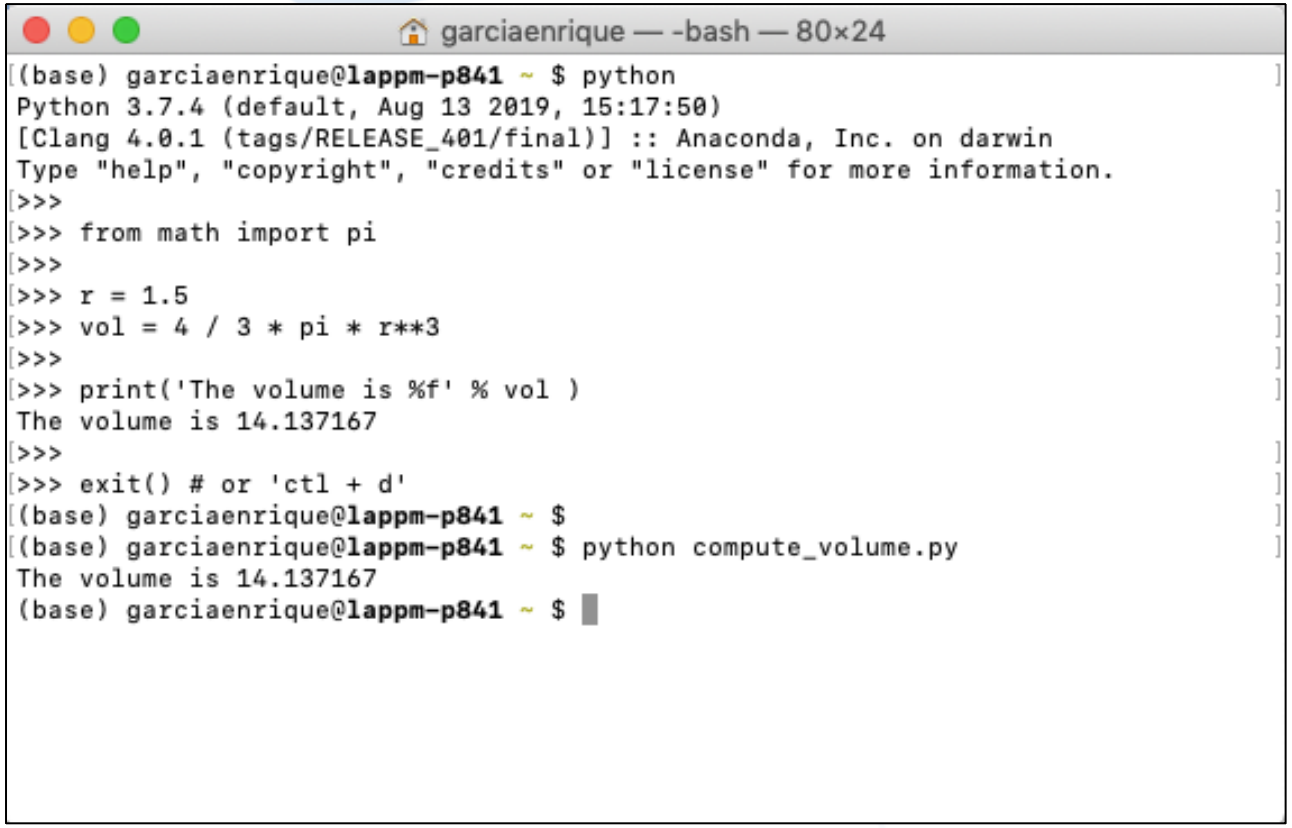
- Python interpreter
  - The engine that runs python
  - Operates like a shell
  - Start it by typing

    `$ python`
  - Exit by typing

    ≫ exit()

- Scripts can be run too (f.ex)

  `$ python script_name.py`



```
[(base) garciaenrique@lappm-p841 ~ $ python
Python 3.7.4 (default, Aug 13 2019, 15:17:50)
[Clang 4.0.1 (tags/RELEASE_401/final)] :: Anaconda, Inc. on darwin
Type "help", "copyright", "credits" or "license" for more information.
[>>>
[>>> from math import pi
[>>>
[>>> r = 1.5
[>>> vol = 4 / 3 * pi * r**3
[>>>
[>>> print('The volume is %f' % vol )
The volume is 14.137167
[>>>
[>>> exit() # or 'ctl + d'
[(base) garciaenrique@lappm-p841 ~ $
[(base) garciaenrique@lappm-p841 ~ $ python compute_volume.py
The volume is 14.137167
(base) garciaenrique@lappm-p841 ~ $ 
```

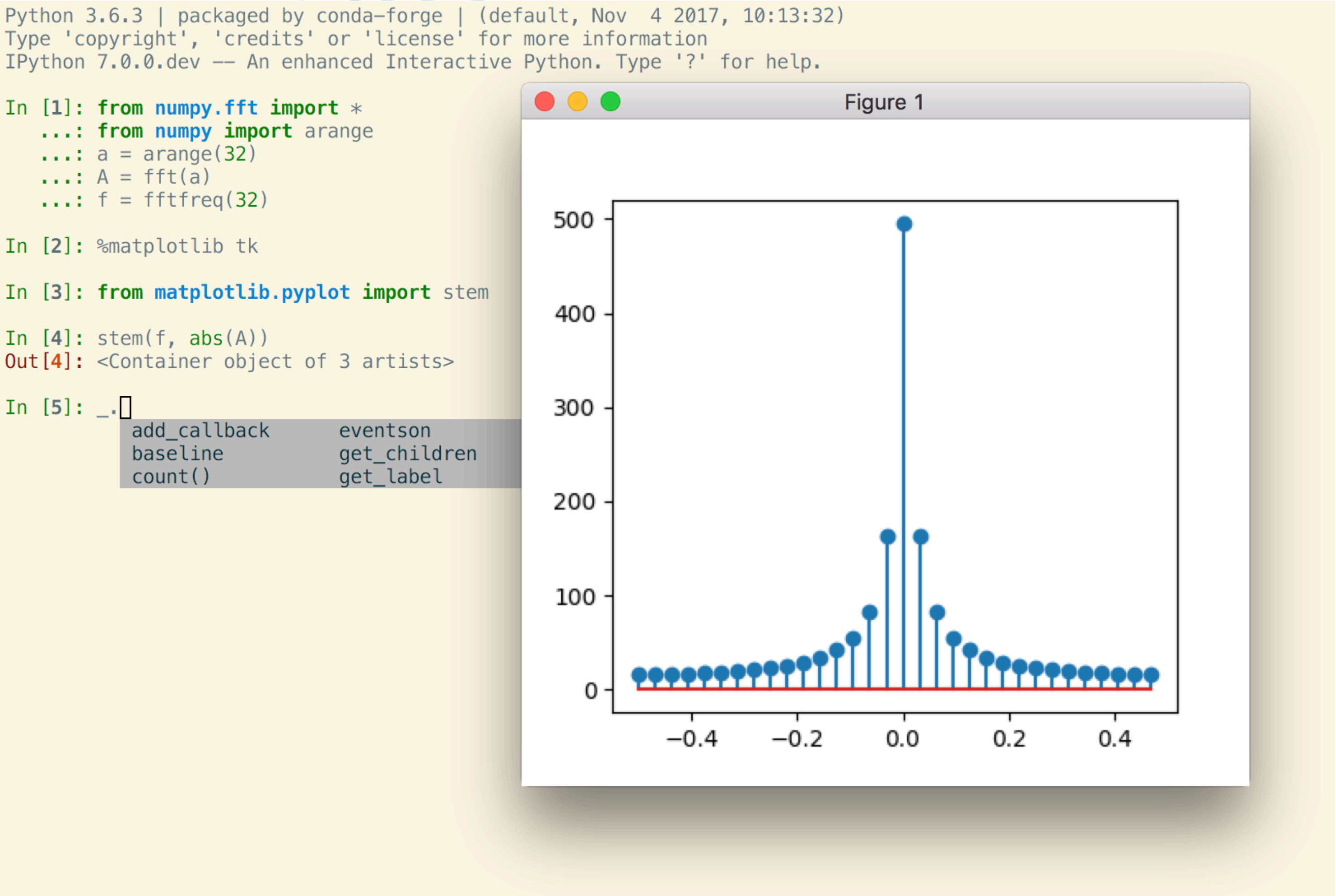
IPython

- More interactive shell and command line
  - Code completion
  - Highlights

- Uses an IPython Kernel – Introduces the concept of ”cell magics”

- Launch it by typing

  `$ ipython`



```
Python 3.6.3 | packaged by conda-forge | (default, Nov  4 2017, 10:13:32)
Type 'copyright', 'credits' or 'license' for more information
IPython 7.0.0.dev -- An enhanced Interactive Python. Type '?' for help.

In [1]: from numpy.fft import *
   ...: from numpy import arange
   ...: a = arange(32)
   ...: A = fft(a)
   ...: f = fftfreq(32)

In [2]: %matplotlib tk

In [3]: from matplotlib.pyplot import stem

In [4]: stem(f, abs(A))
Out[4]: <Container object of 3 artists>

In [5]: _.
          add_callback        eventson
          baseline            get_children
          count()             get_label
```

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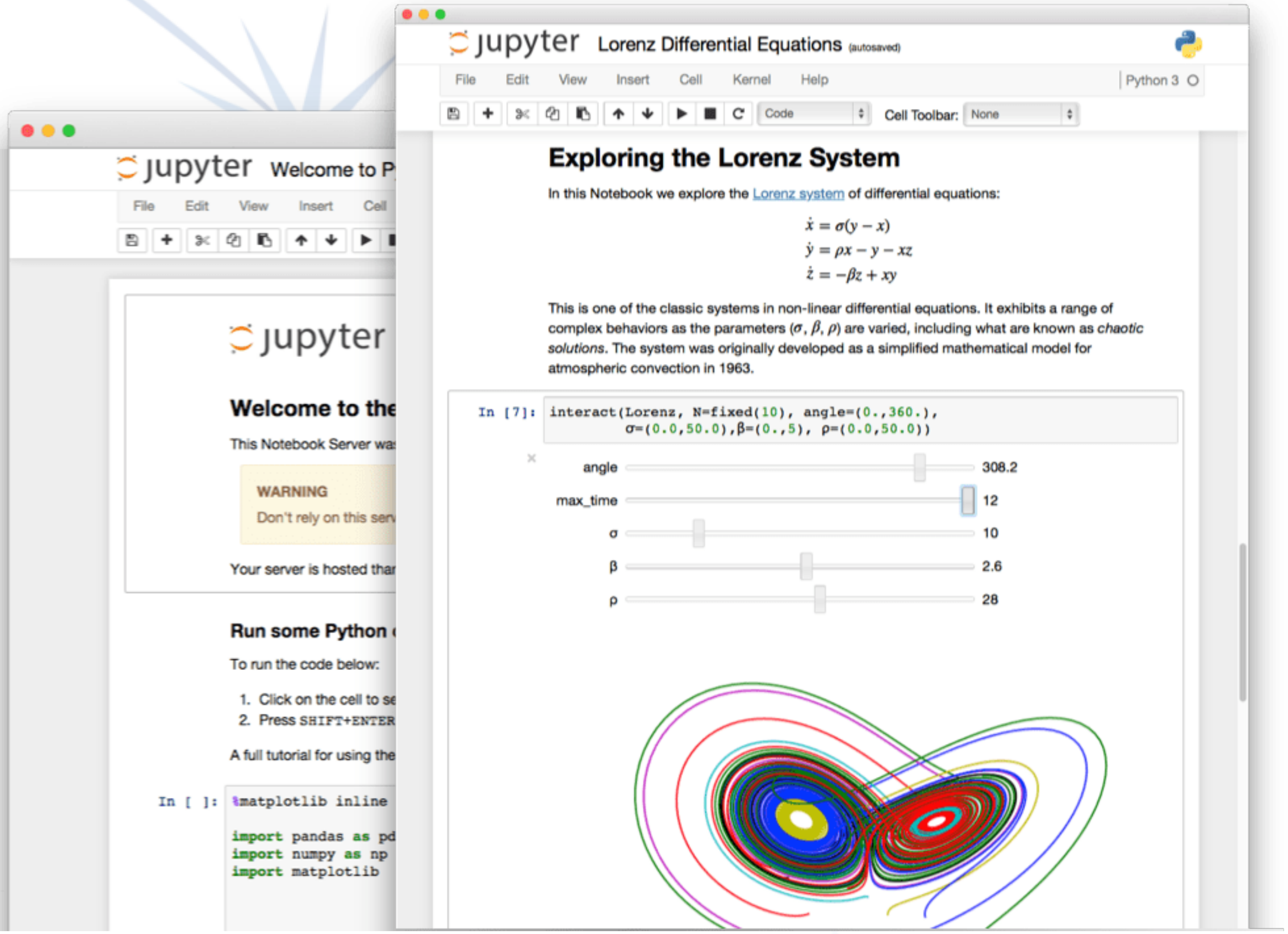
Jupyter Notebook

- Side project of the IPython project, that originally contained an IPython notebook project also.

- Why Jupyter ?
  - Core supported languages Julia, Python and R



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Run some Python

To run the code below:

1. Click on the cell to se
2. Press SHIFT+ENTER

A full tutorial for using the

```
In [ ]: %matplotlib inline

        import pandas as pd
        import numpy as np
        import matplotlib
```

Exploring the Lorenz System

In this Notebook we explore the Lorenz system of differential equations:

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = \rho x - y - xz$$
$$\dot{z} = -\beta z + xy$$

This is one of the classic systems in non-linear differential equations. It exhibits a range of complex behaviors as the parameters (σ, β, ρ) are varied, including what are known as *chaotic solutions*. The system was originally developed as a simplified mathematical model for atmospheric convection in 1963.

```
In [7]: interact(Lorenz, N=fixed(10), angle=(0.,360.),
                 σ=(0.0,50.0),β=(0.,5), ρ=(0.0,50.0))
```

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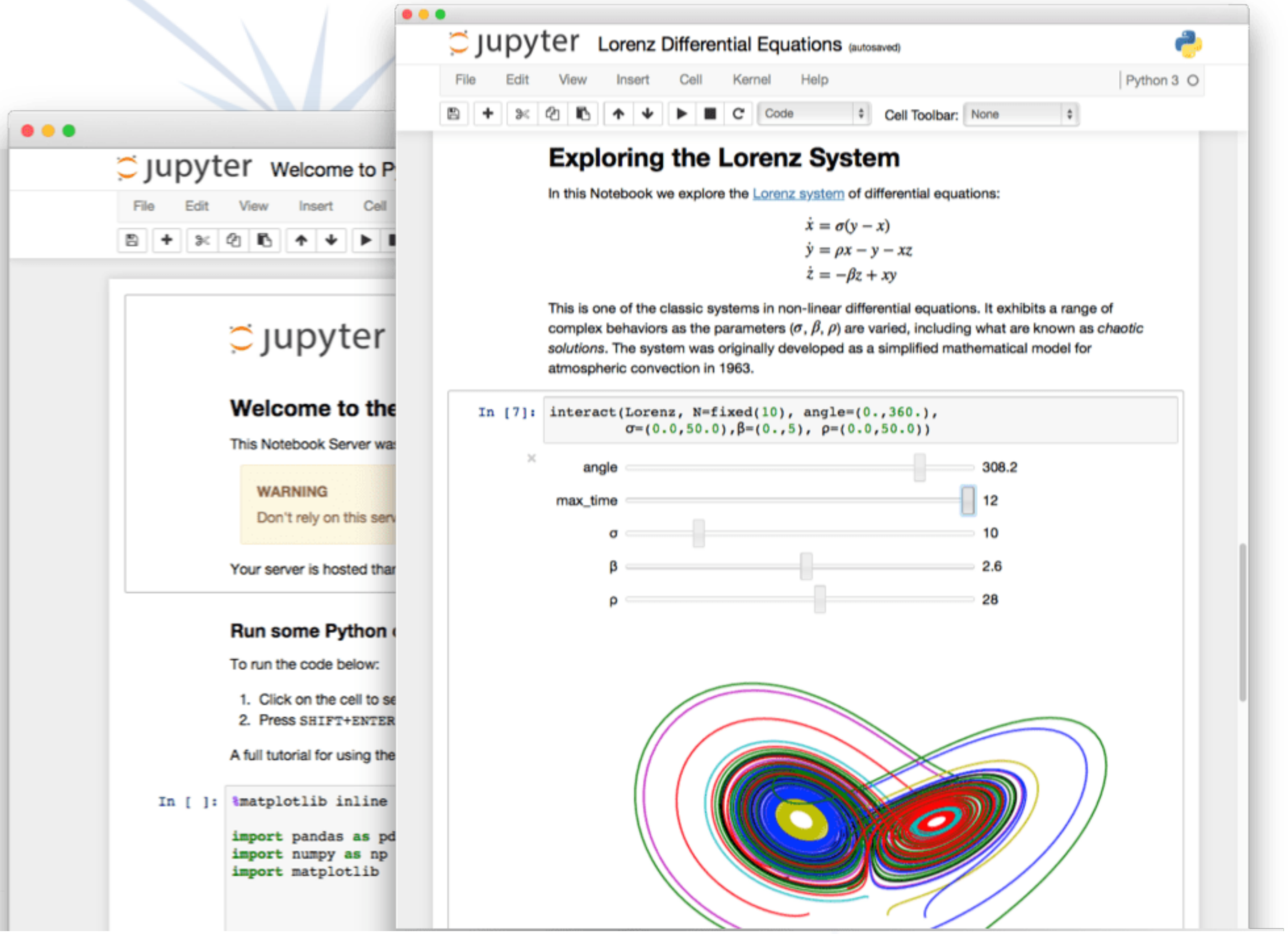
Jupyter Notebook

- How do we create/run one ?
  - .ipynb files

- Notebook interface
  - Cells
  - Cell types
  - Kernels



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Lorenz Differential Equations (autosaved)

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```

angle 308.2
max_time 12
σ 10
β 2.6
ρ 28

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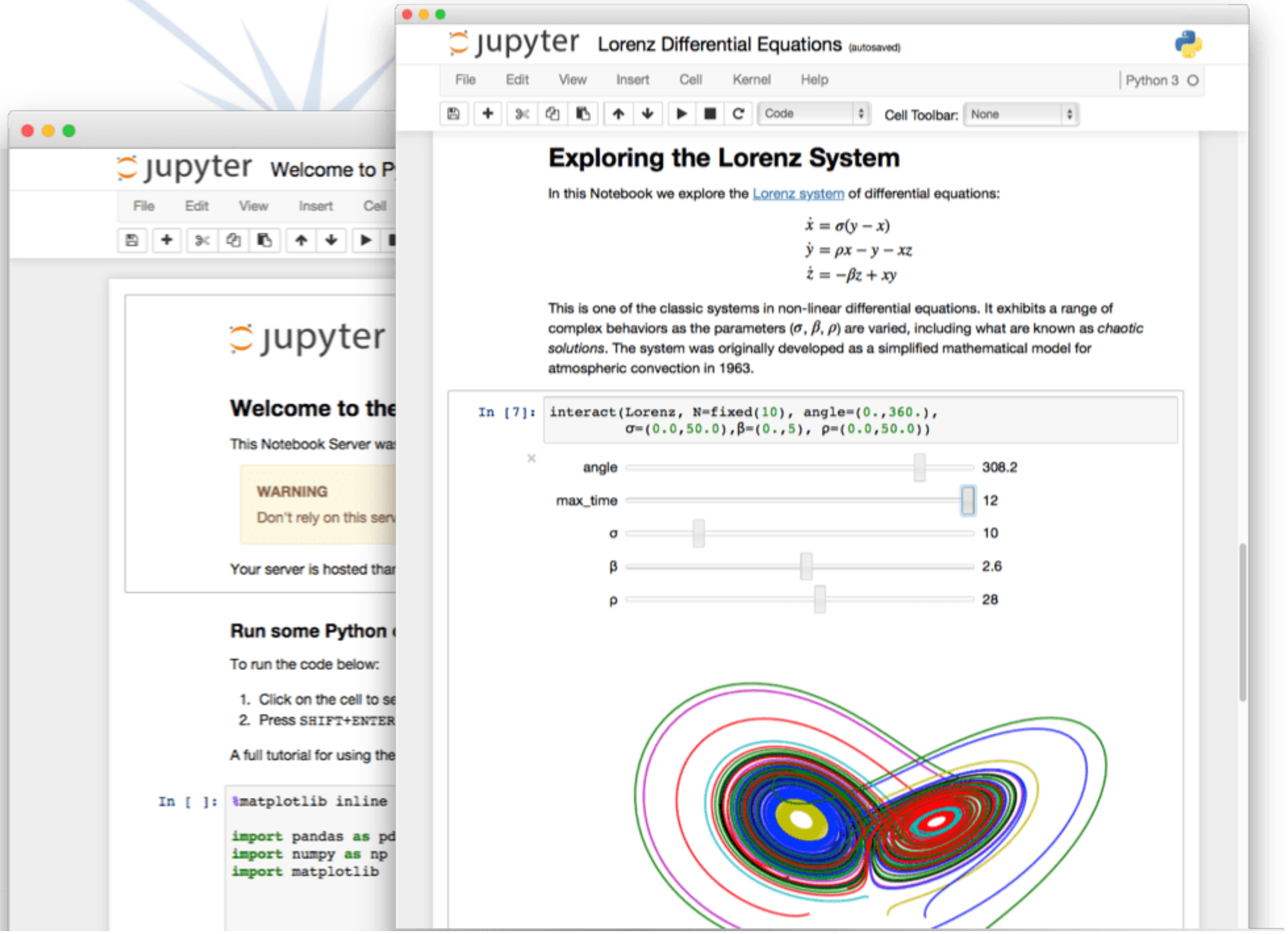
Jupyter Notebook

- How to share a notebook:
  - GitHub
  - NBViewer

  - ipynb file can be exported to
    - HTML
    - LaTeX
    - PDF
    - Markdown
    - An executable script
    - ReStructured Text
    - RevealJS

```
$ Jupyter nbconvert <input_notebook.ipynb> --to <output format>
```



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Jupyter Notebook

- Advanced features and useful functionalities to present results
  - Jupyter Widgets
  - Hiding the code
  - Creating a presentation with Jupyter Notebooks

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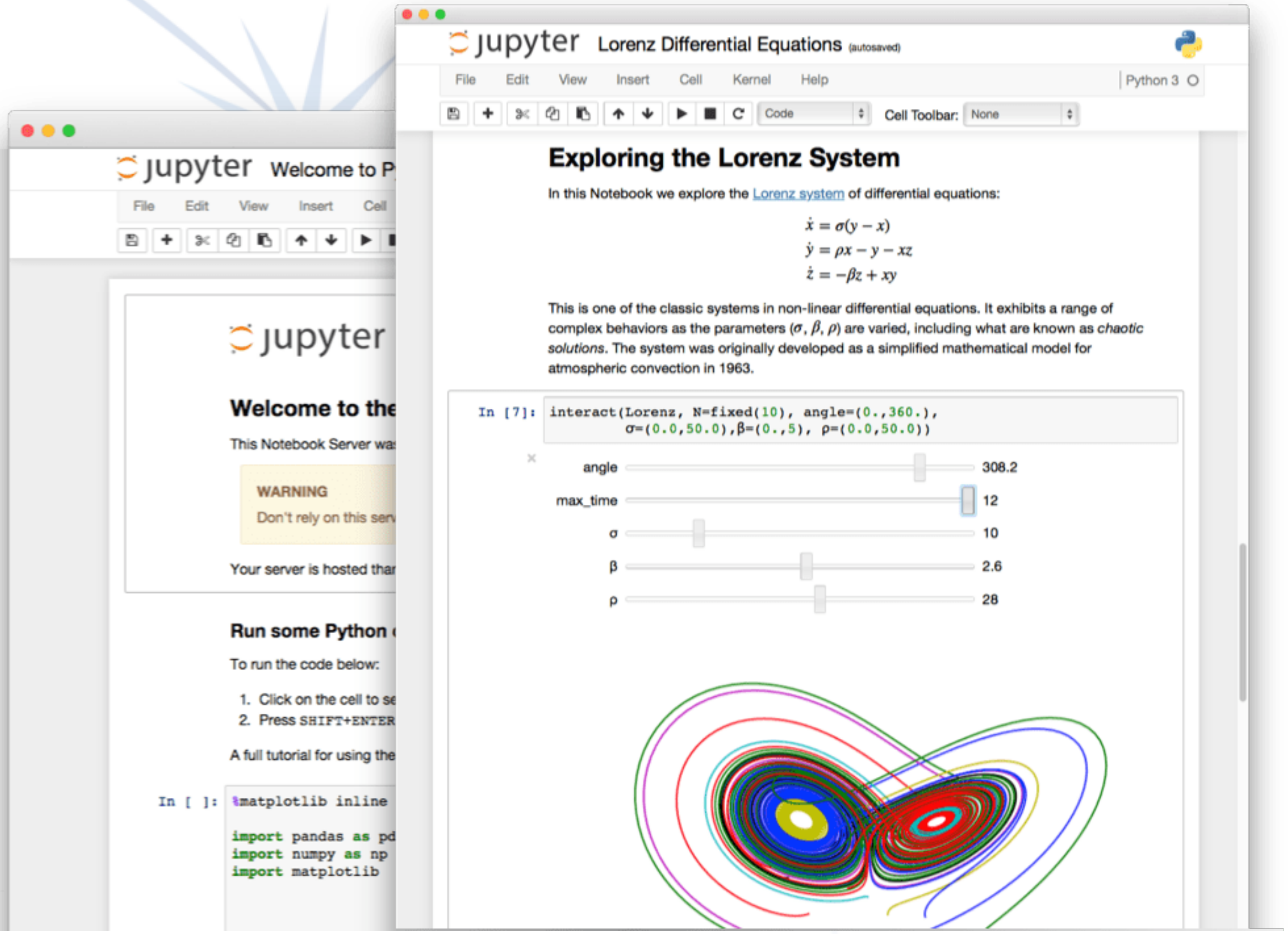
Jupyter Notebook

- Nice tool to
  - (quick) Exploratory analysis
  - Nice way to present results*
    - Markdown + code

- Maybe not that optimal to
  - Develop
  - Show results in between large amounts of code



jupyter

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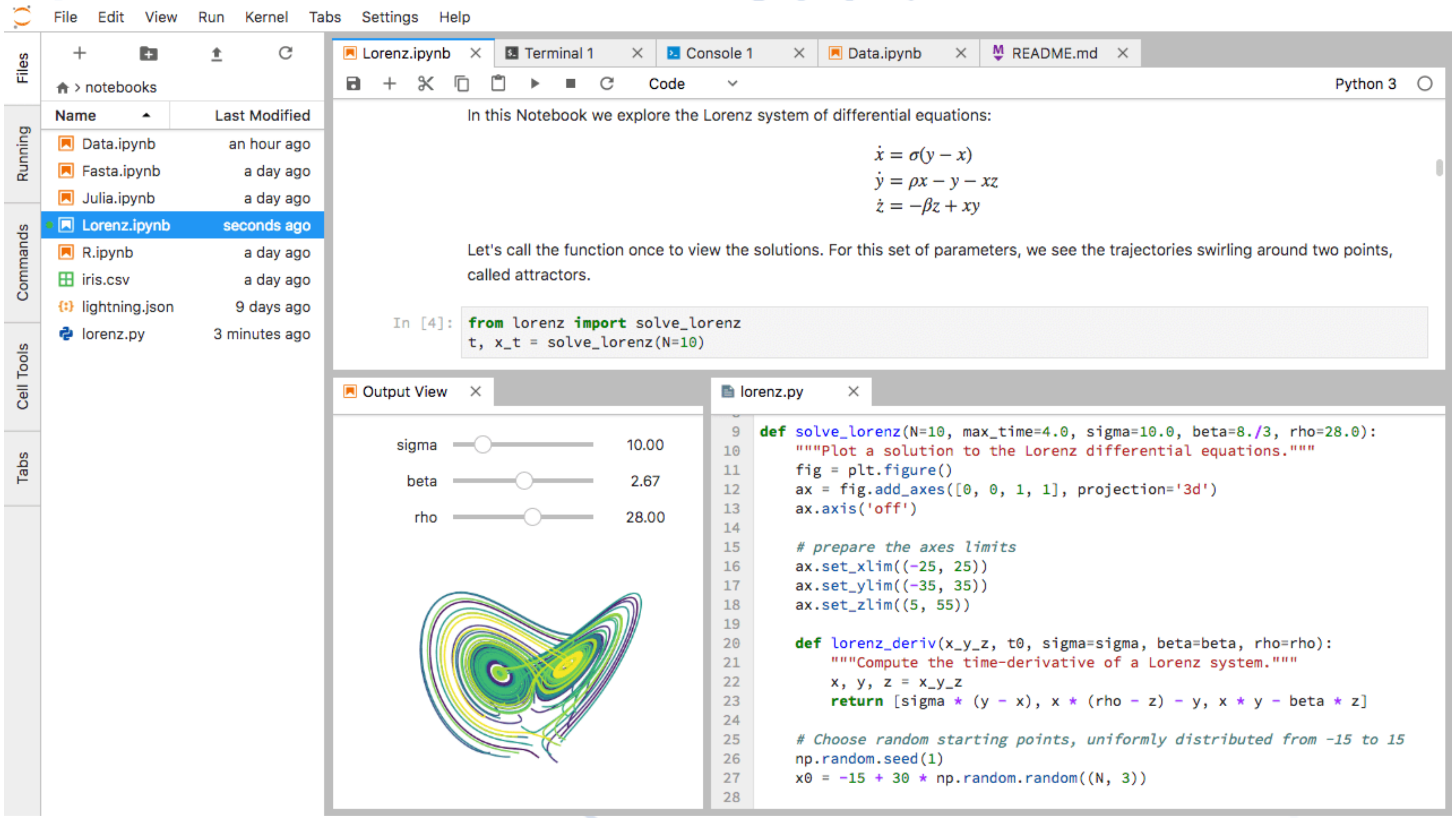
Jupyter Lab



Name	Last Modified
Data.ipynb	an hour ago
Fasta.ipynb	a day ago
Julia.ipynb	a day ago
Lorenz.ipynb	seconds ago
R.ipynb	a day ago
iris.csv	a day ago
lightning.json	9 days ago
lorenz.py	3 minutes ago

In this Notebook we explore the Lorenz system of differential equations:

$$\begin{aligned}\dot{x} &= \sigma(y - x)\\ \dot{y} &= \rho x - y - xz\\ \dot{z} &= -\beta z + xy\end{aligned}$$

Let's call the function once to view the solutions. For this set of parameters, we see the trajectories swirling around two points, called attractors.

```
In [4]: from lorenz import solve_lorenz
        t, x_t = solve_lorenz(N=10)
```

sigma 10.00

beta 2.67

rho 28.00

```python
def solve_lorenz(N=10, max_time=4.0, sigma=10.0, beta=8./3, rho=28.0):
    """Plot a solution to the Lorenz differential equations."""
    fig = plt.figure()
    ax = fig.add_axes([0, 0, 1, 1], projection='3d')
    ax.axis('off')

    # prepare the axes limits
    ax.set_xlim((-25, 25))
    ax.set_ylim((-35, 35))
    ax.set_zlim((5, 55))

    def lorenz_deriv(x_y_z, t0, sigma=sigma, beta=beta, rho=rho):
        """Compute the time-derivative of a Lorenz system."""
        x, y, z = x_y_z
        return [sigma * (y - x), x * (rho - z) - y, x * y - beta * z]

    # Choose random starting points, uniformly distributed from -15 to 15
    np.random.seed(1)
    x0 = -15 + 30 * np.random.random((N, 3))

```

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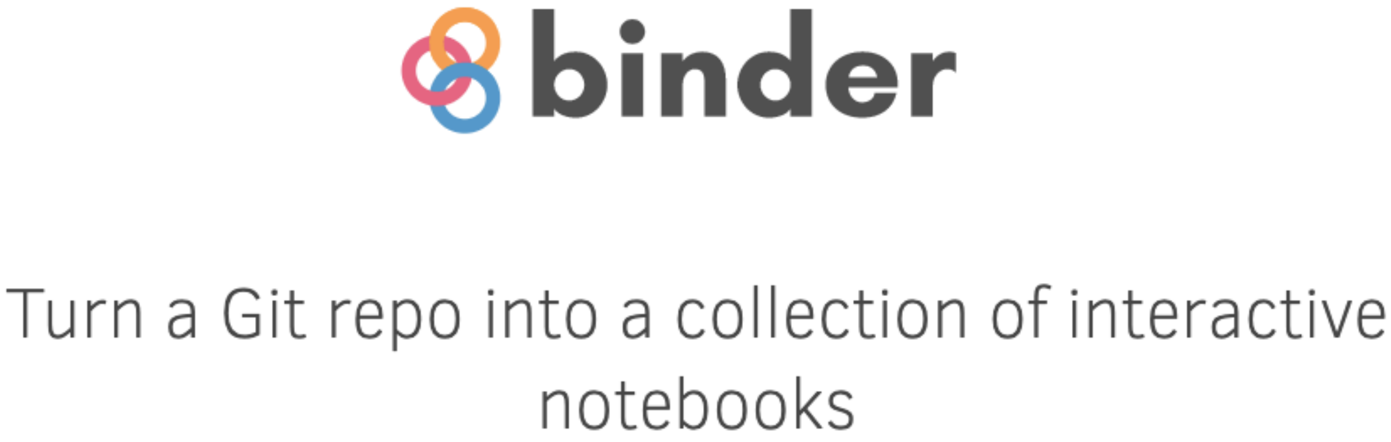
Binder

- Interactive notebooks from a single click !
- Builds a Docker image of the repository
  - by installing all the dependencies within the environment.yml file



binder

Turn a Git repo into a collection of interactive notebooks

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Thank your for your attention

- Links and sources
  - IPython (Slide 5): IPython tutorial https://nbviewer.jupyter.org/github/ipython/ipython/blob/6.x/examples/IPython%20Kernel/Index.ipynb
  - NBViwer (Slide 8): https://nbviewer.jupyter.org/
  - Binder (Slide 12): https://mybinder.org/
  - Jupyter Notebooks:
    - Tutorials and links inside notebooks

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