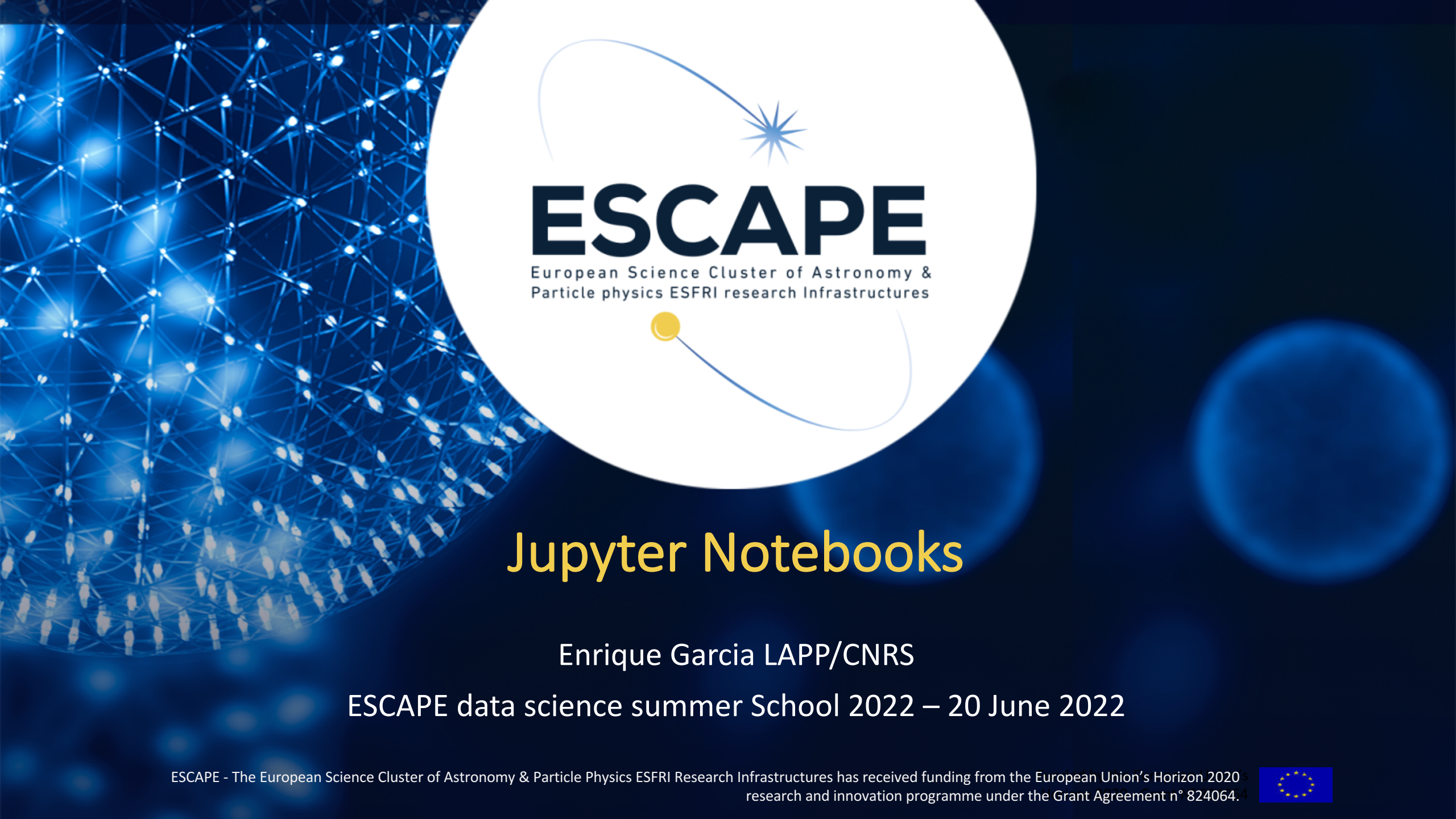

Jupyter Notebooks

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ESCAPE data science summer School 2022 – 20 June 2022

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Overview

- Python
- IPython
- Jupyter
  - Jupyter Notebooks
    - Basic usage
    - Useful features for presenting results
  - JupyterLab
- Reproducible computer environments
  - Binder
  - Docker

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Python

- Multi purpose
  - Like C, C++ or Java, it is designed to build software in a variety of domains
- Interpreted
  - Code does not need to be previously compiled
- Object oriented (OOP)
  - Code is designed around data (objects) that contains properties and attributed
  - ”Contrary” to Imperative (C), functional (SQL, Mathematica…) or logic programming
- High-level
  - Independent of type of computer

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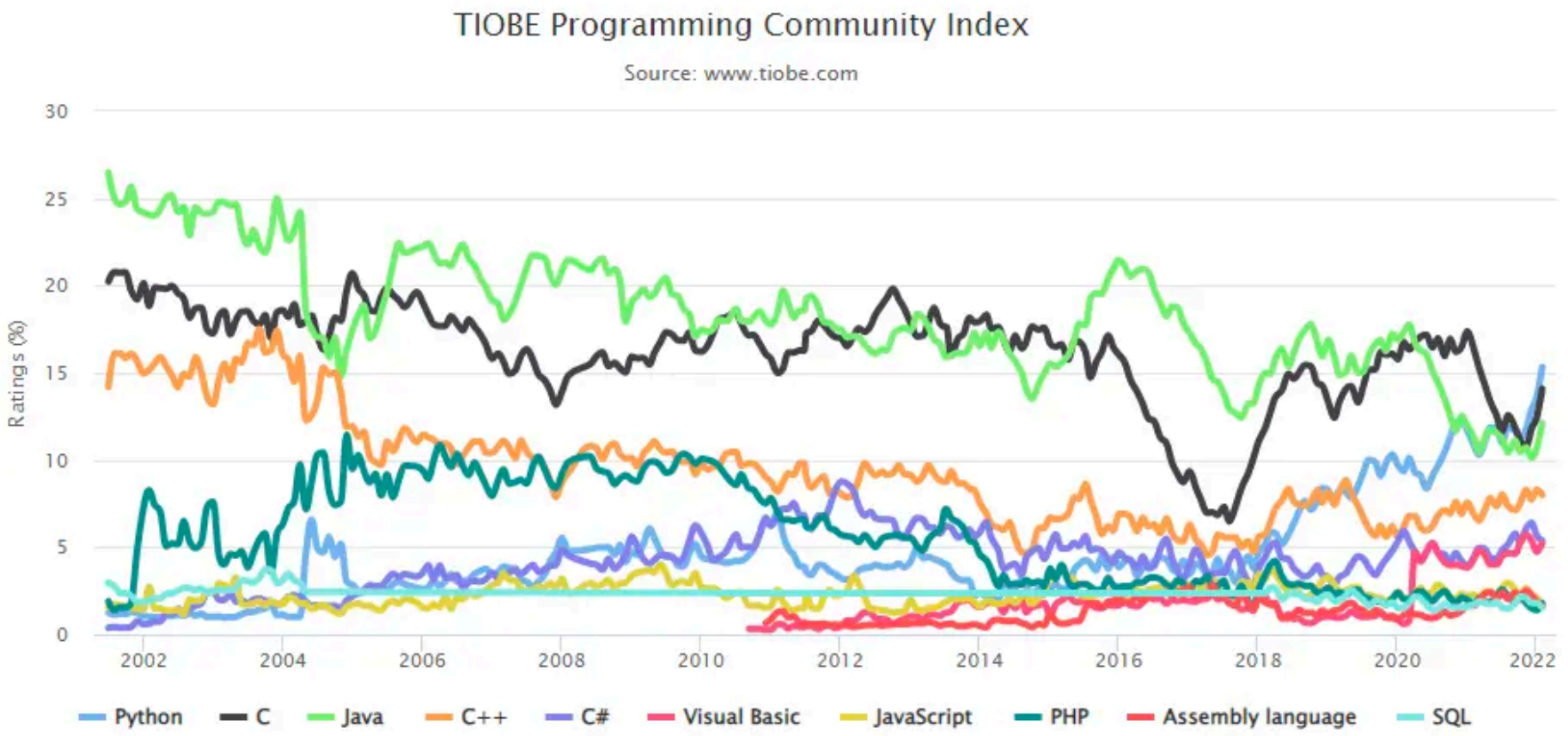
Python

- Released in 1991
- Python 1.0 released in 1994.
  - Guido Van Rossum
- Python 2 was released in 2000 and Python 3 in 2008.
  - Python2.7
  - Python3.10



- Currently one of the most used programming languages.

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Python

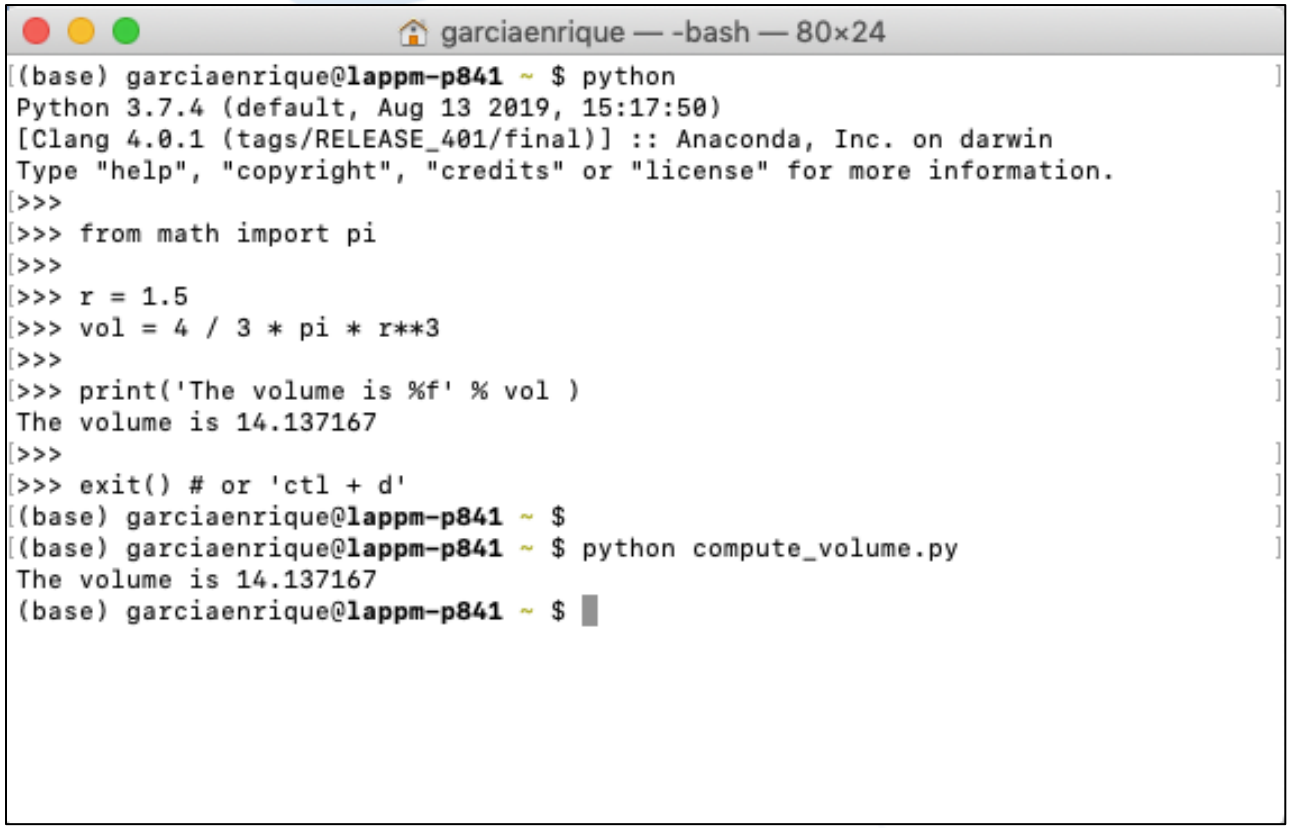
- Python interpreter
  - The engine that runs python
  - Operates like a shell
  - Start it by typing

    `$ python`
  - Exit by typing

    » exit()

- Scripts can be run too (f.ex)

  `$ python script_name.py`



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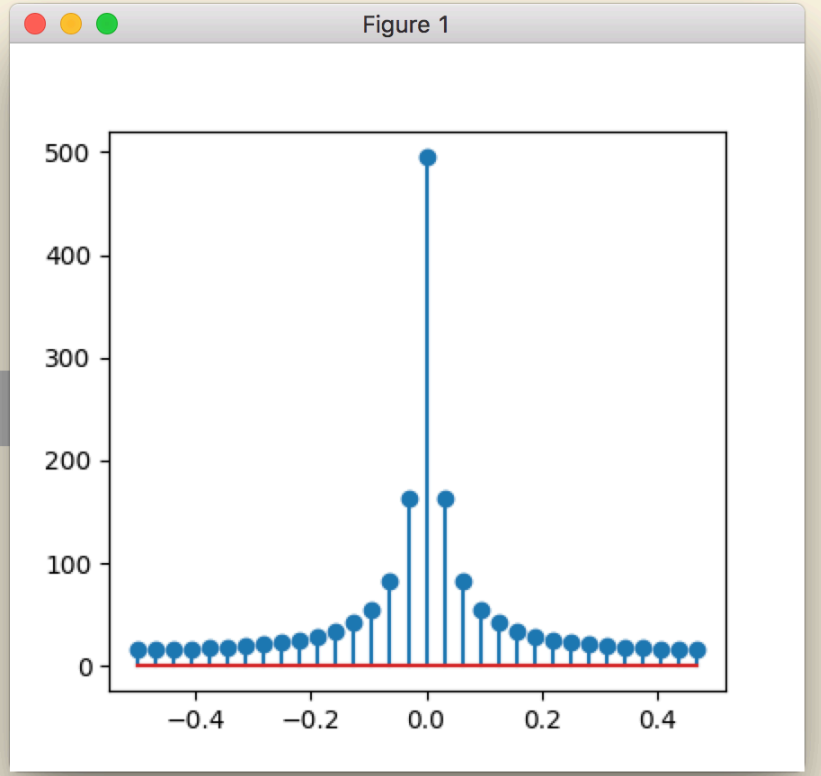
IPython

- More interactive shell and command line
  - Code completion
  - Highlights
  - Visualisation tools (GUIs)
  - ”cells and scripts magics”
- Uses an IPython Kernel
  - The python interpreter (backend)
  - Default kernel in Jupyter project
- 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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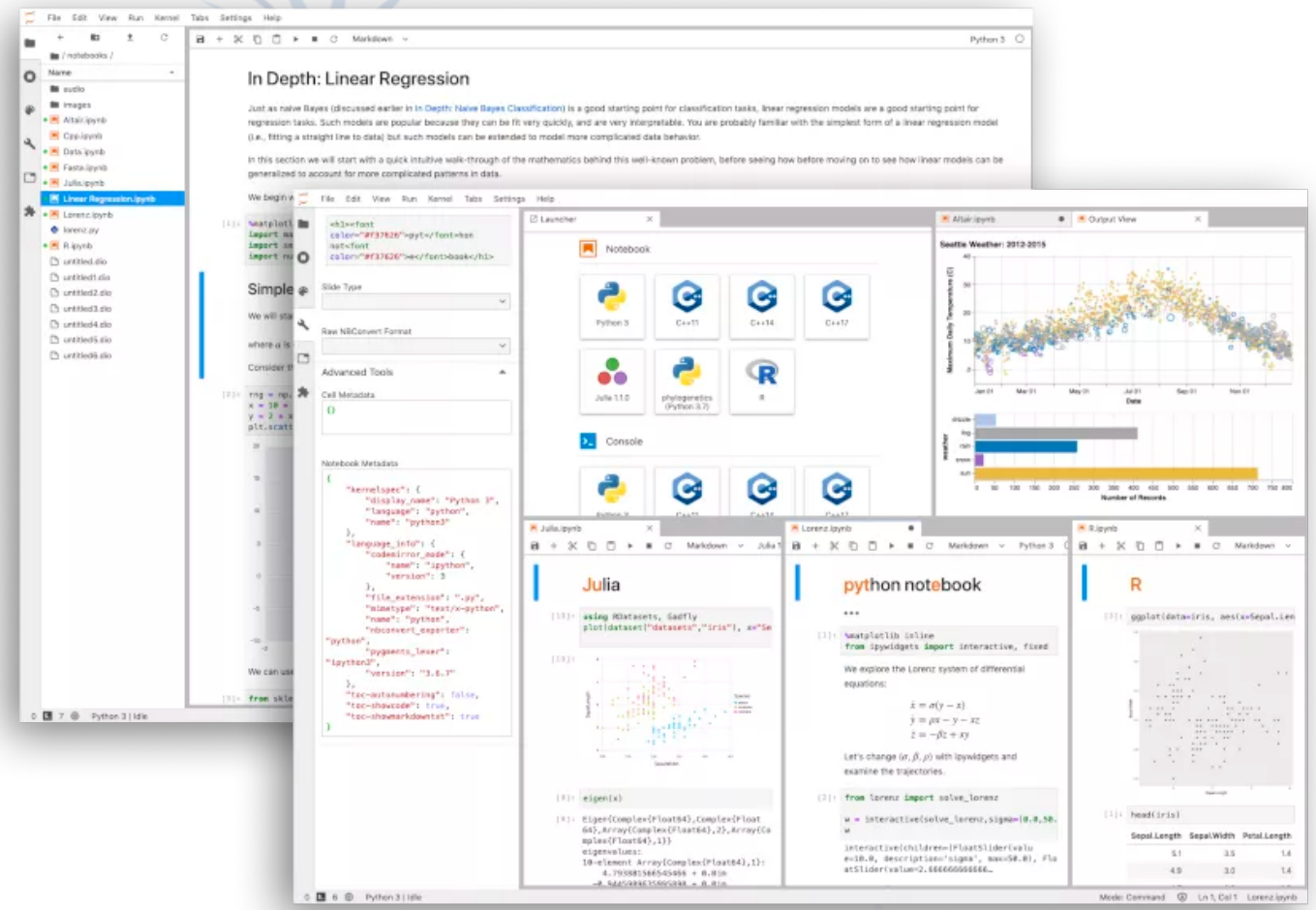
Jupyter (project)

- Side project of the IPython project
  - Started on 2014
  - Included support to
    - **Ju**lia, **Py**thon, **R** (Jupyter)
- Web based computing platform that mixes
  - Code and equations and text,
  - Visualization environment and tools…
  - File manager
- Interfaces:
  - Jupyter Notebook
  - JupyterLab



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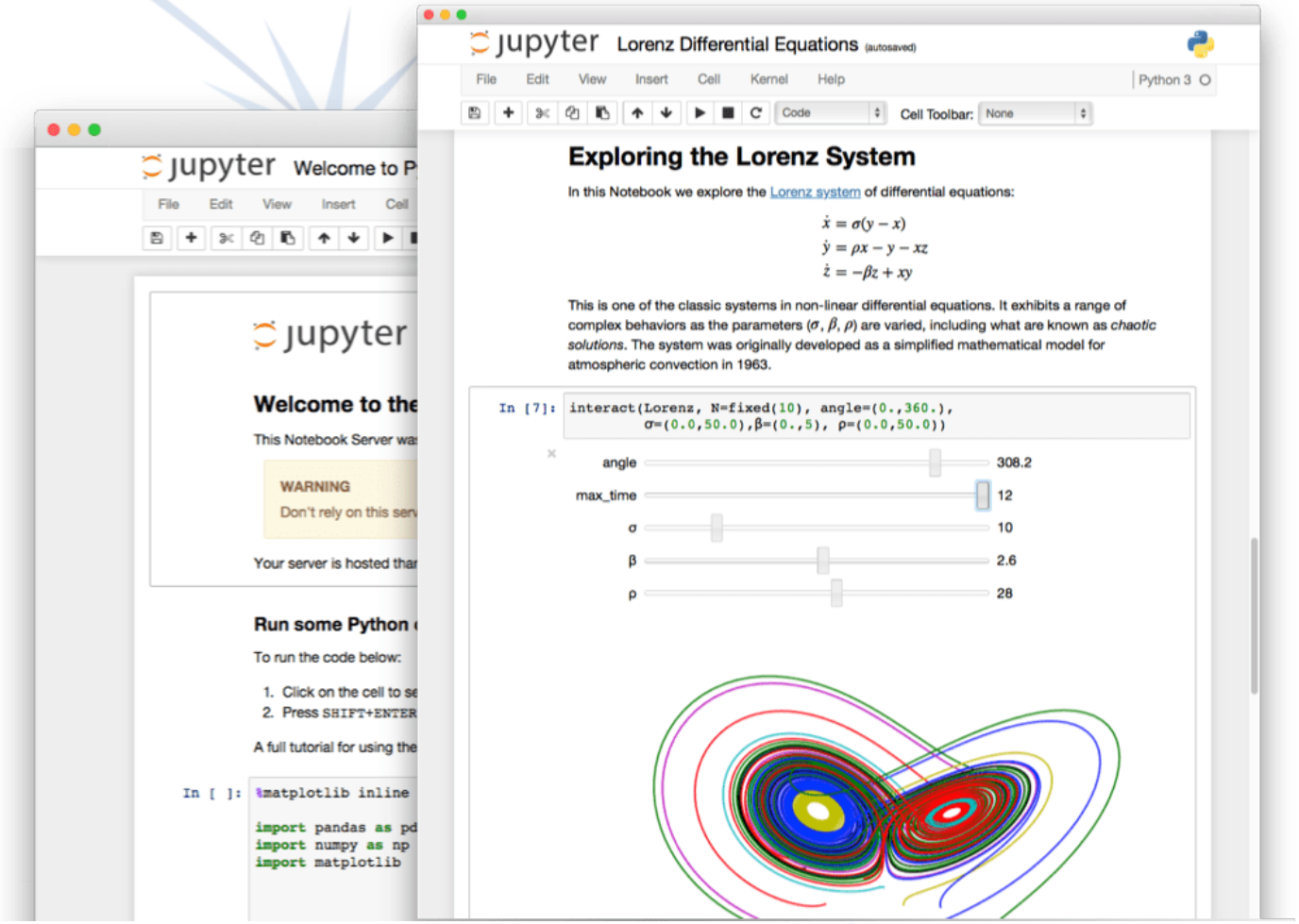
Jupyter Notebook

- Tutorial & Demo
  - How to create and run a jupyter Notebook
  - Interface: Cell types
  - How to share/export a notebook
  - How to install other Kernels
- Advanced features
  - Jupyter Widgets
  - Hiding the code
  - Creating a presentation with Jupyter Notebooks



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Jupyter Notebook

- Installing other kernels:

- Julia

  - Download Julia

```
$ conda install julia
```

  - Launch Julia

```
$ julia
julia> using Pkg
julia> Pkg.add("Ijulia")
julia> exit()
```

  - Launch a new Jupyter session

- R

  - Download R
    - `conda install -c r r-irkernel`

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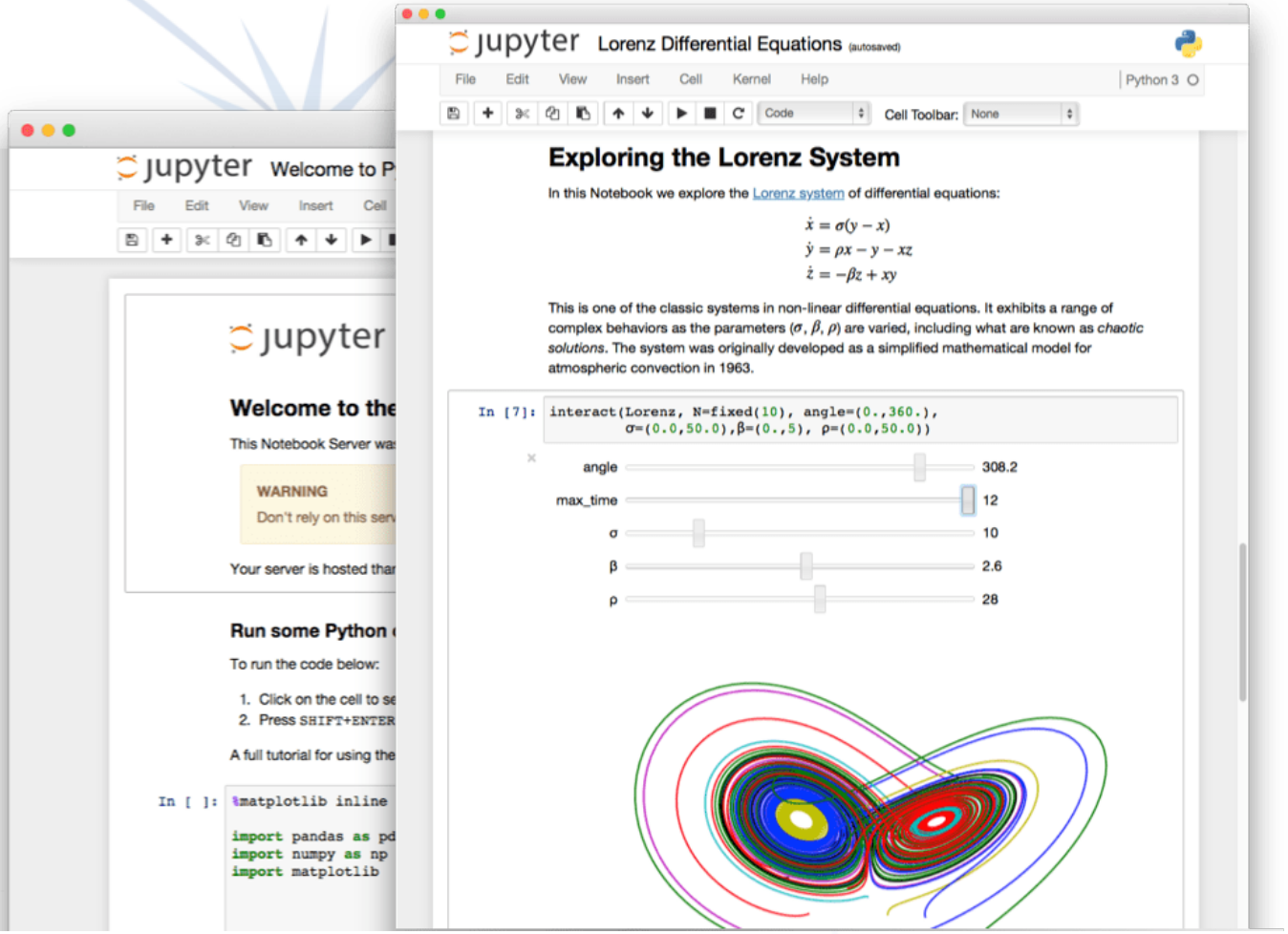
Jupyter Notebook

- How to share a notebook:
  - GitHub/GitLab
  - NBViewer: https://nbviewer.org/

- An 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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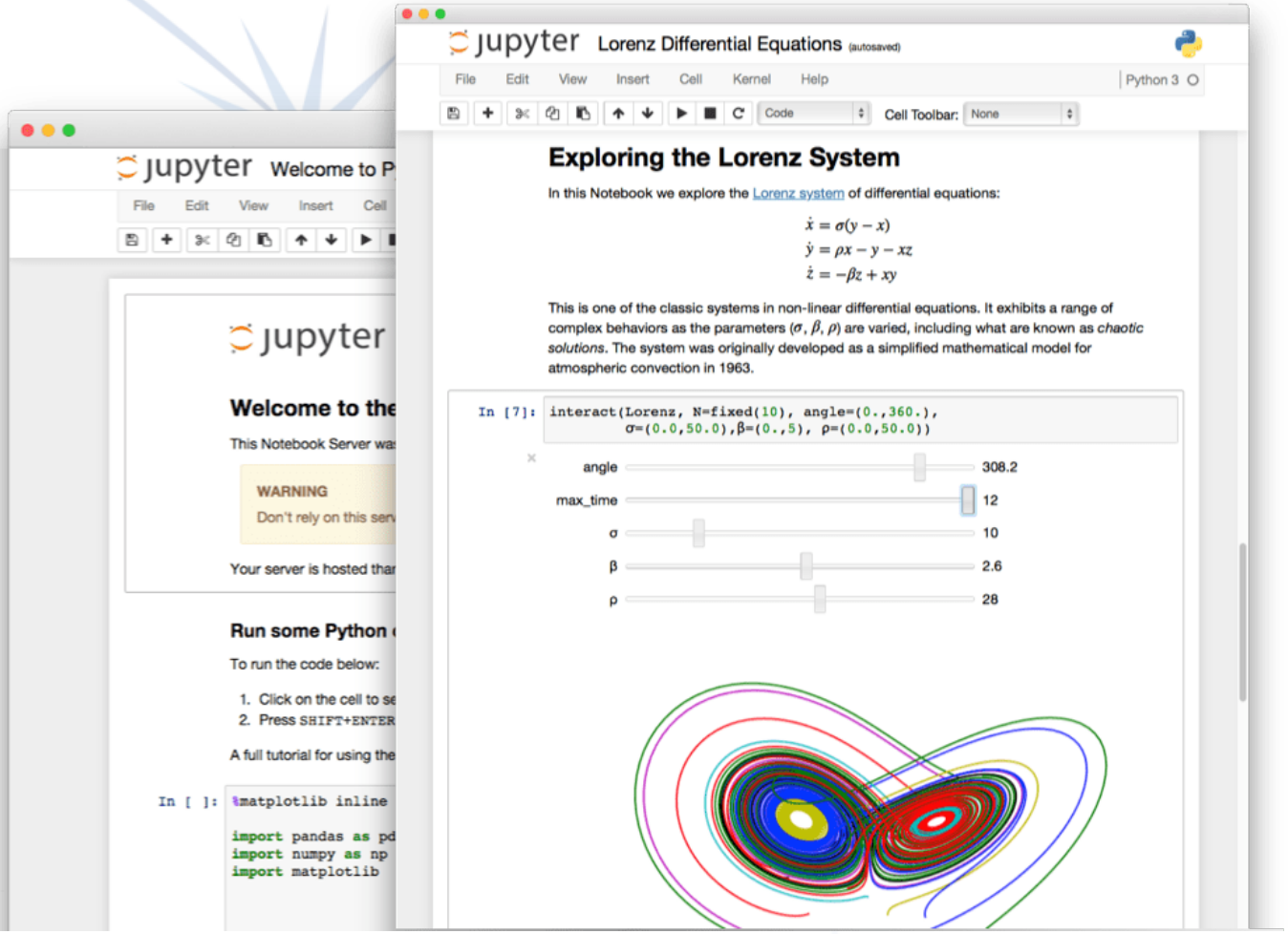
Jupyter Notebook

- 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



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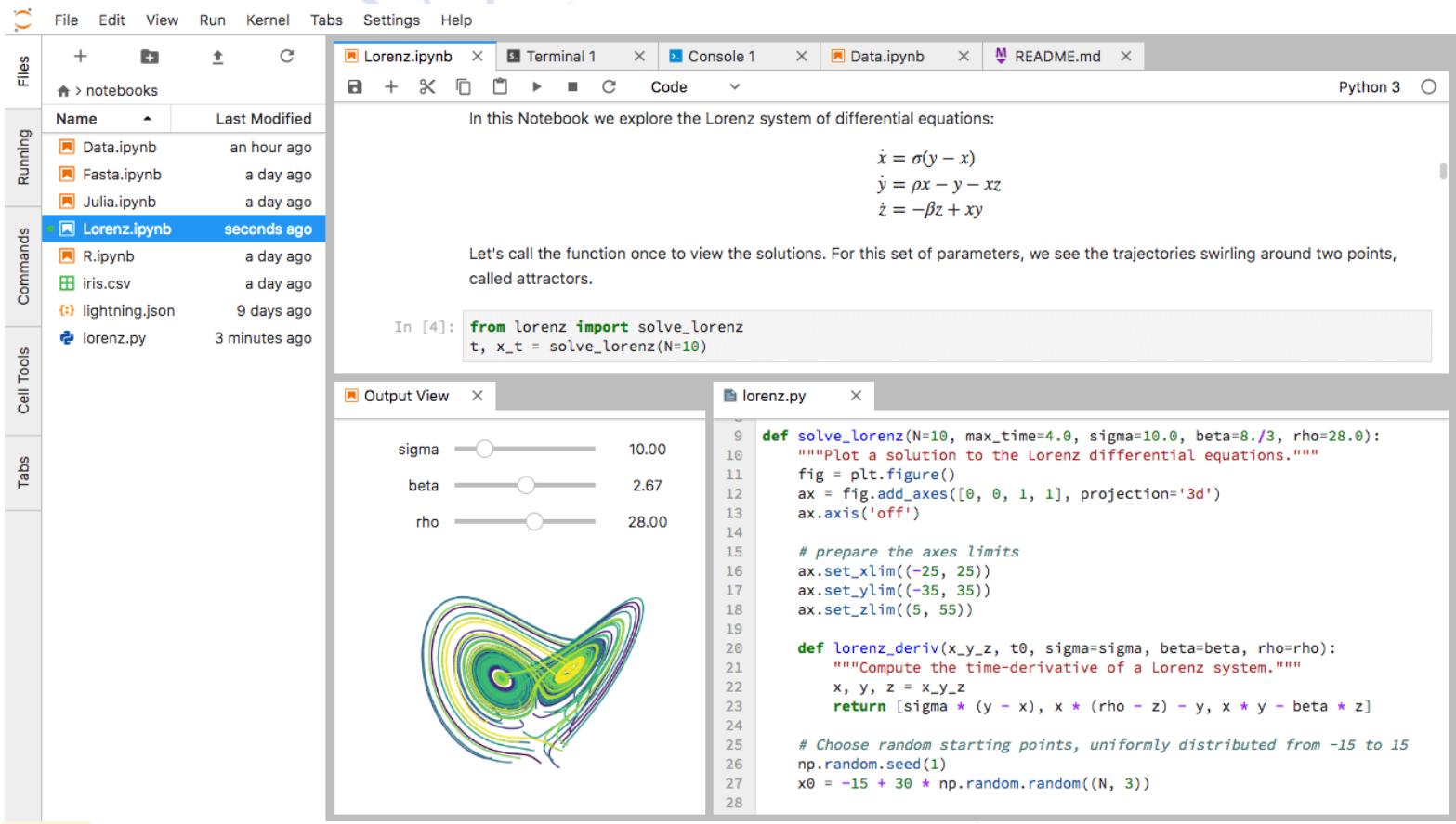
Jupyter Lab

- Interactive and modular web-based environment
  - Includes same functionalities Jupyter notebooks
  - File manager
  - Launcher of Jupyter interfaces

- Launch it

```
$ jupyter-lab
```



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Reproducible computer environments

Turn a Git repo into a collection of interactive notebooks

https://mybinder.org/

- Builds and runs a docker container of the repository
  - by installing all the dependencies within the `environment.yml file`

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Docker

- Application that virtualizes software packages into a ”container”.
  - The resulting file is called a **docker image**
  - When executing an image, you are running a **docker container**
  - Other virtualisation alternatives: Singularity, Podman...

- How to install Docker ?
  - Recommendation, use docker desktop: https://docs.docker.com/get-docker/

- Pros:
  - Portability
  - Reproducibility
- Cons:
  - Leaning curve

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Docker

- Downloading and running the school image

```
$ docker pull ghcr.io/escape2020/escape-datascience-school2022:latest
$ docker run -p 8888:8888 ghcr.io/escape2020/escape-datascience-school2022:latest
```


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Reproducible computer environments

- This was possible thanks to the use of **open science,** some of its tools and following FAIR principles

  - An open github project – version control + Zenodo record (Findable) (Accessible)
  - A file describing the **computer environment** (Interoperable)
    - conda: environment.yml
    - Python: requirements.txt
  - A **public license** + The use of open source CI/CD tools (Reusable)

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Thank your for your attention

Any question or comment ?

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