Jupyter Notebooks 101

A Reproducible Research Workshop

Simon Stone
Research Data Services
Dartmouth College

• Reproducible Research @ DARTMOUTH

About the Reproducible Research Group

- Joint venture of **Research Computing @ ITC** and **Research Data Services @ Library**
- Consult with **experts** on
  - research data management,
  - data visualization,
  - biomedical research support,
  - spatial data and GIS,
  - high performance and research computing,
  - statistical analysis,
  - economics and social sciences data
- **Meet** the people on campus that support your reproducible research lifecycle
- **Engage** in community discussions to learn from other researchers on campus
- Attend a workshop to **learn** practical tools and tips

About Research Data Services

Research Data Management

Data Management Plans (DMPs) for sponsored projects

Finding and using 3rd party data

Collection and cleaning of data

Organization and documentation

Publishing and Repositories

Data Analysis/Visualization

Textual, numeric, spatial data

Reproducible research workflows

Scripting in R: tidyverse core package (i.e. ggplot, dplyr, tydr, tibble, etc.)

Scripting in Python: NumPy, SciPy, Pandas, Scikit-learn, Matplotlib, Seaborn, (OpenCV, PyTorch, TensorFlow, Tesseract, NLTK, etc.)

Computational Scholarship

Computational project planning

Collections as Data

Storytelling with data and visualizations

Text and data mining

Digital Humanities support

Computational Pedagogy

Work with us

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Why talk about Jupyter Notebooks?

- ☝️ Jupyter Notebooks are an important tool in computational research and education
- ⏭️ Many beginner courses use them, but only gloss over how they work
- 😵‍💫 With only a superficial grasp of them, Jupyter Notebooks can get in the way of learning and understanding
- 😈 Some bad practices may be unwittingly adopted because of them

What you will learn in this workshop

- **What** are Jupyter Notebooks
- **How** do you use Jupyter Notebooks
- **What to look out for** when working with Jupyter Notebooks
- **When to use** Jupyter Notebooks

What we will work with in this workshop

- **Jupyter Notebooks** 🎉
- We will use a smattering of **Python** for illustrative code examples
- Materials: **www.dartgo.org/rr-notebooks101**

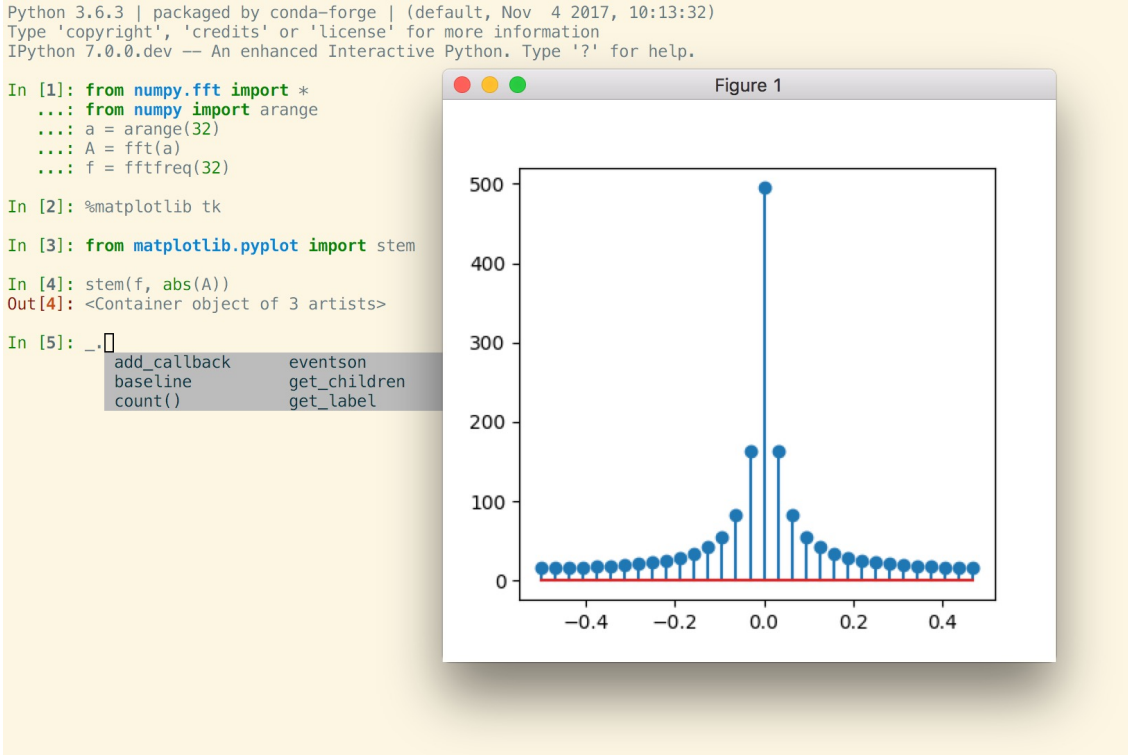
Let’s get started…

A brief history of Jupyter

In 2001, Fernando Pérez wanted a better Python shell

He created IPython:

- Syntax highlighting
- Autocompletion
- Interactive visualizations



A brief history of Jupyter

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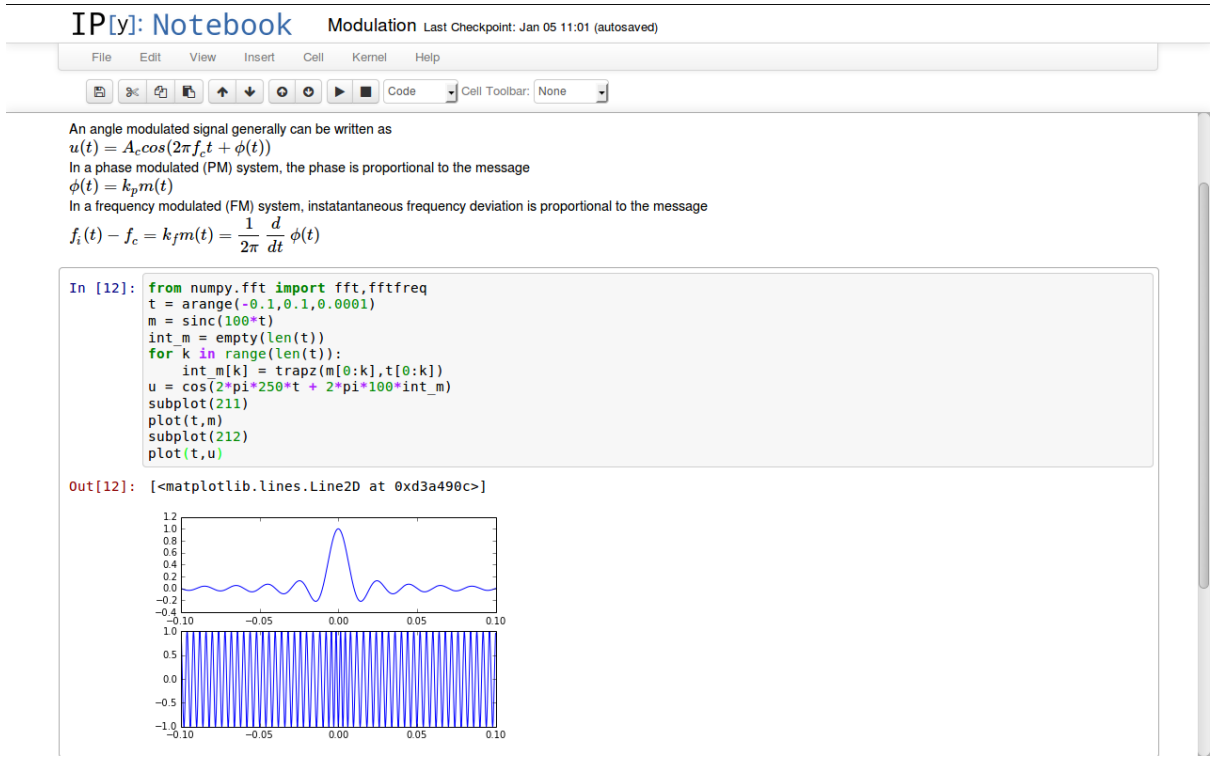
He created IPython:

- Syntax highlighting
- Autocompletion
- Interactive visualizations
- A rich editor view mixing text, code, and visualizations



A brief history of Jupyter

- In 2014, Pérez and his team realized that their editor functionality in IPython was actually independent of the programming language used
- Project Jupyter was spun off from IPython
- Jupyter: Julia, Python, R
  (the originally supported languages)

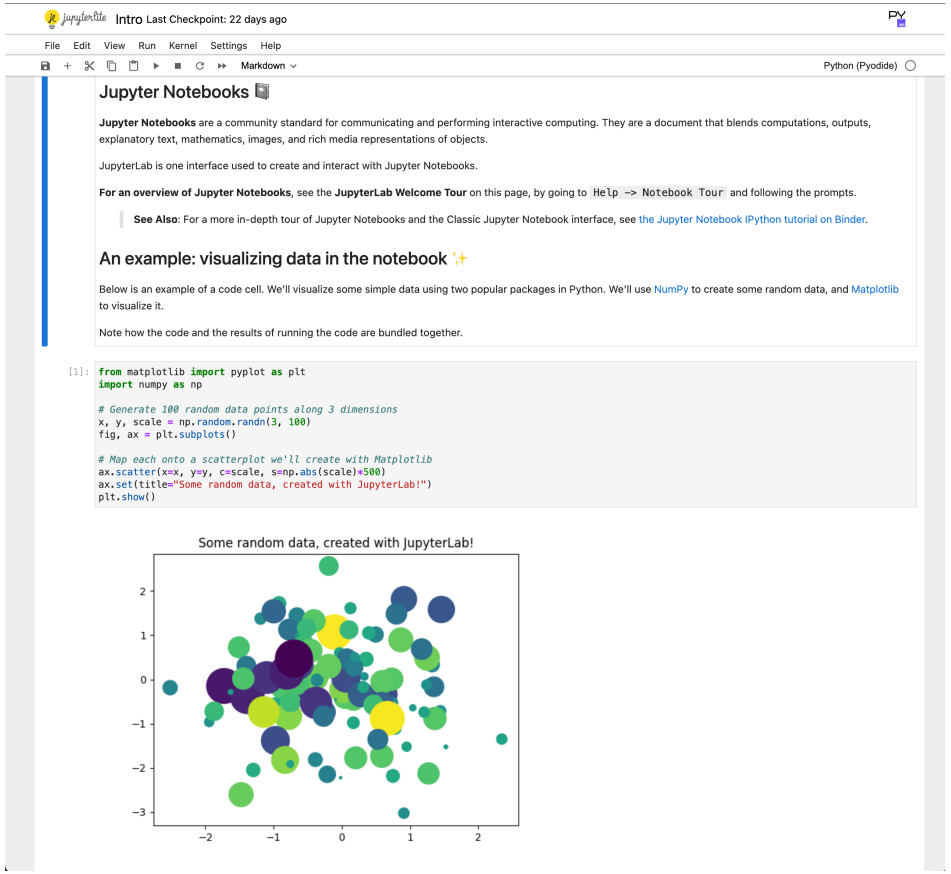
Cameron Oelsen, BSD, via Wikimedia Commons

- Today, Jupyter Notebooks are used by all major cloud providers
  (Amazon Sagemaker, Google Colaboratory, Microsoft Azure Notebook)
- Jupyter Notebooks are virtually *everywhere* in research and education
- *The Atlantic:* "The Scientific Paper is Obsolete"

What is a Jupyter Notebook?

Source: https://jupyter-notebook-beginner-guide.readthedocs.io/en/latest/what_is_jupyter.html

- Notebooks are files produced by the Jupyter Notebook application, which contain both computer code (e.g., python) and rich text elements (paragraph, equations, figures, links, etc…).
- The Jupyter Notebook App is a server-client application that allows editing and running notebook files via a web browser.
- The Jupyter Notebook App can be executed on a local desktop requiring no internet access or can be installed on a remote server and accessed through the internet.



Source: https://jupyter.org/try

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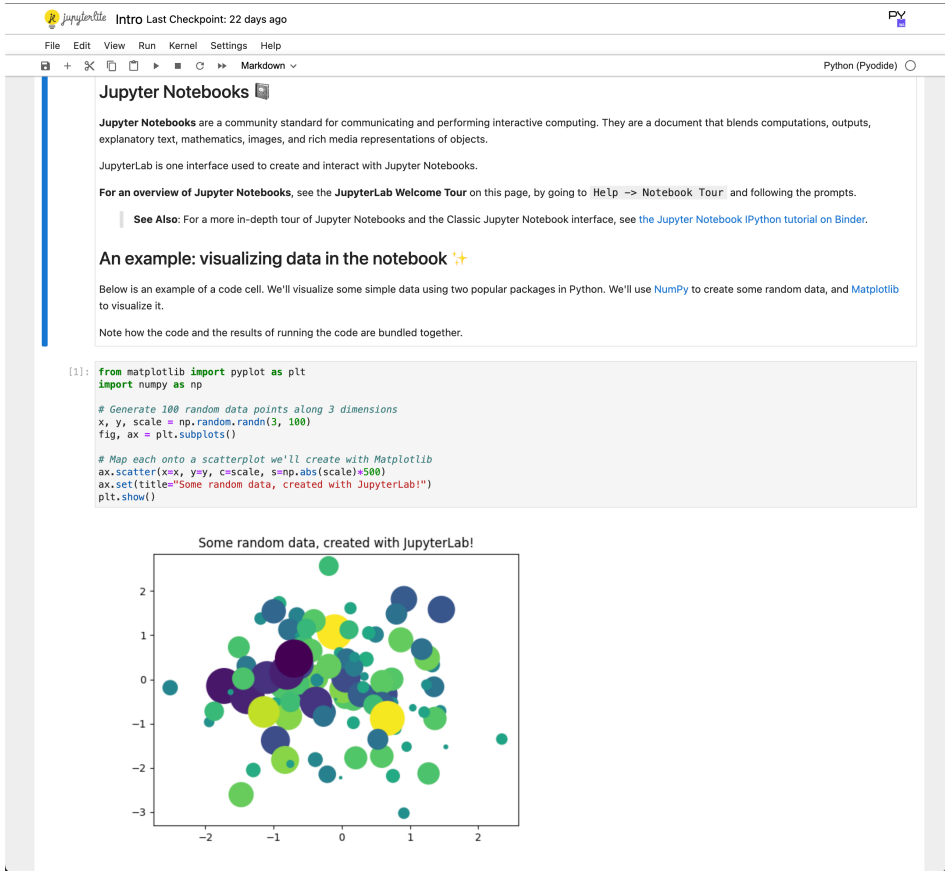
- The code cells are executed by the *kernel,* a computational engine associated with the notebook
- There are many different kernels, each one offering a different programming language:
  - IPython, IRKernel, IJulia, Xeus (C++), many more
- Think of a kernel as a service that your notebook uses to run the code
- The kernel can run on your local machine or remotely (e.g., in the cloud or on an HPC cluster)



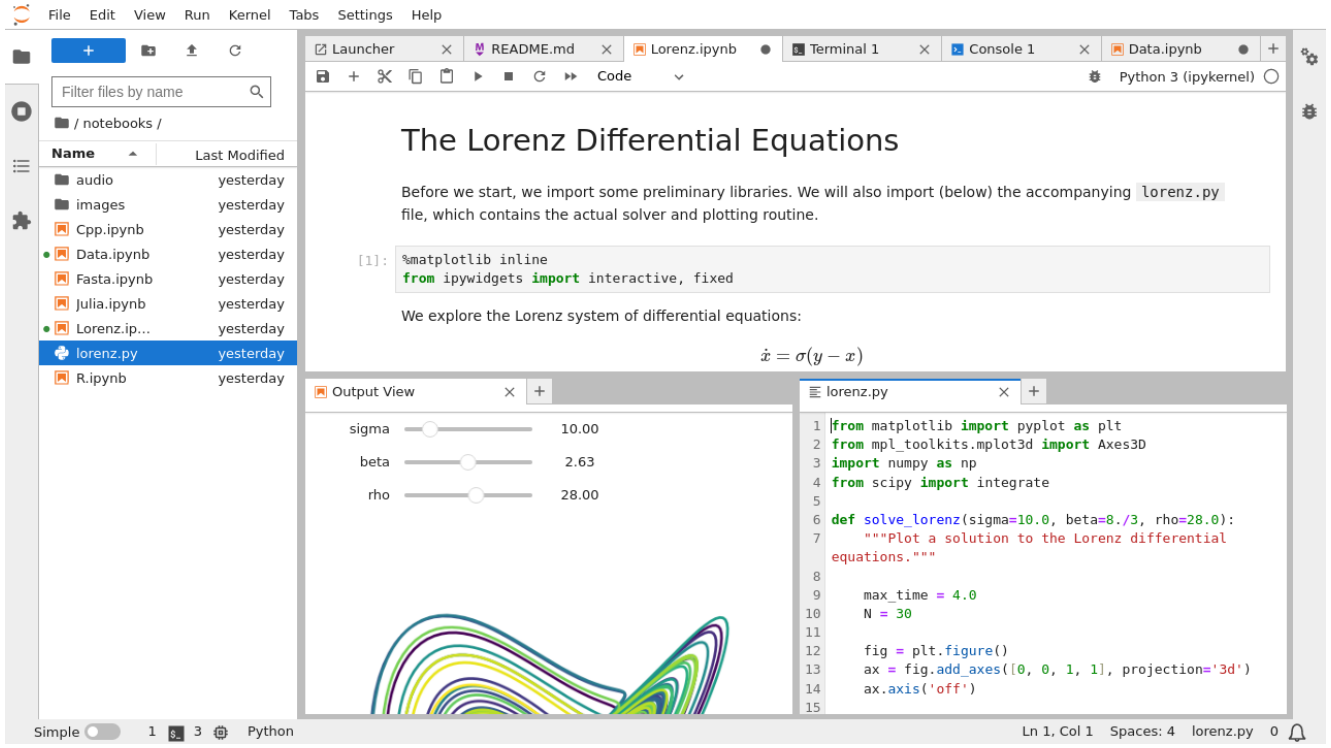
Source: https://jupyter.org/try

How can you run Jupyter Notebooks?

Many ways lead to Jupyter, e.g.:

The official website (www.jupyter.org/install)

- The original Jupyter Notebook App
- The face-lifted, latest version JupyterLab



Source: https://jupyterlab.readthedocs.io/en/latest/

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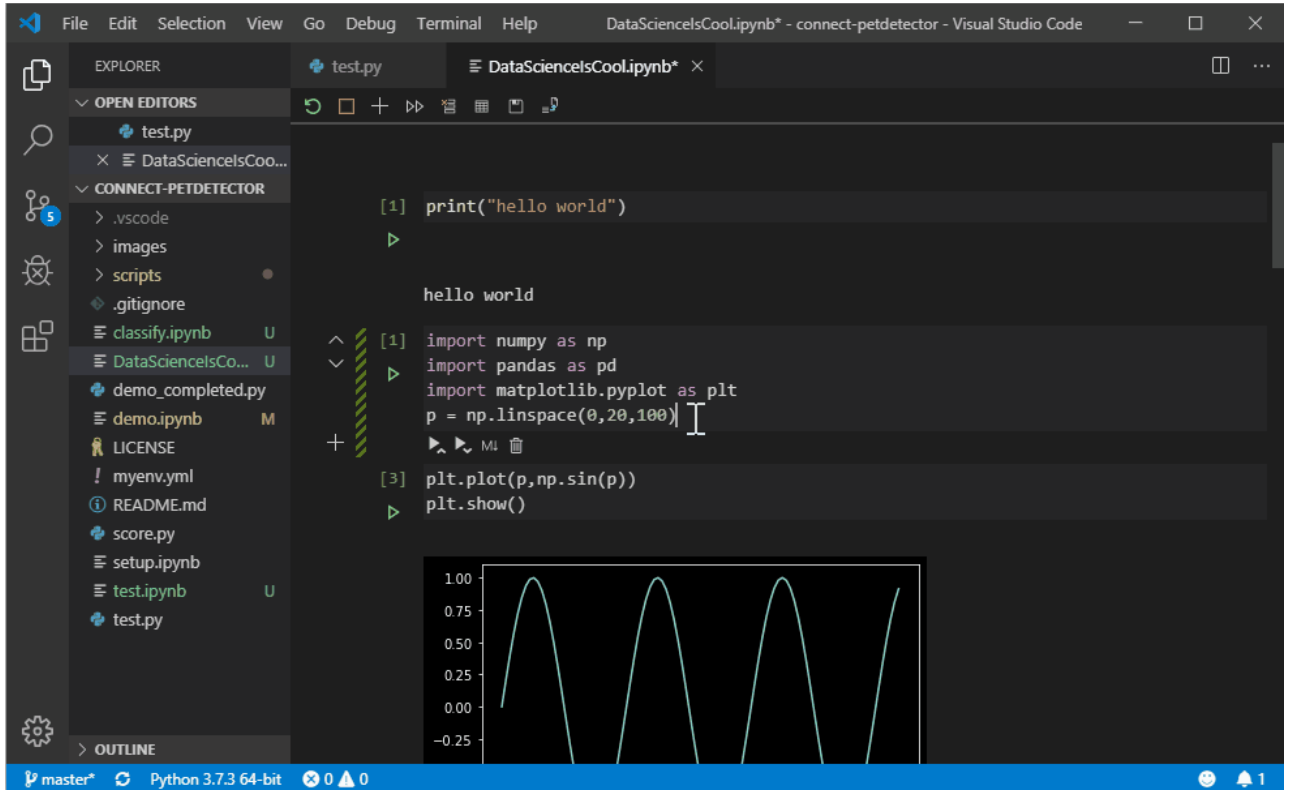
Using a Code Editor/IDE

- E.g., PyCharm or Visual Studio Code



Source: https://towardsdatascience.com/jupyter-notebook-in-visual-studio-code-3fc21a36fe43

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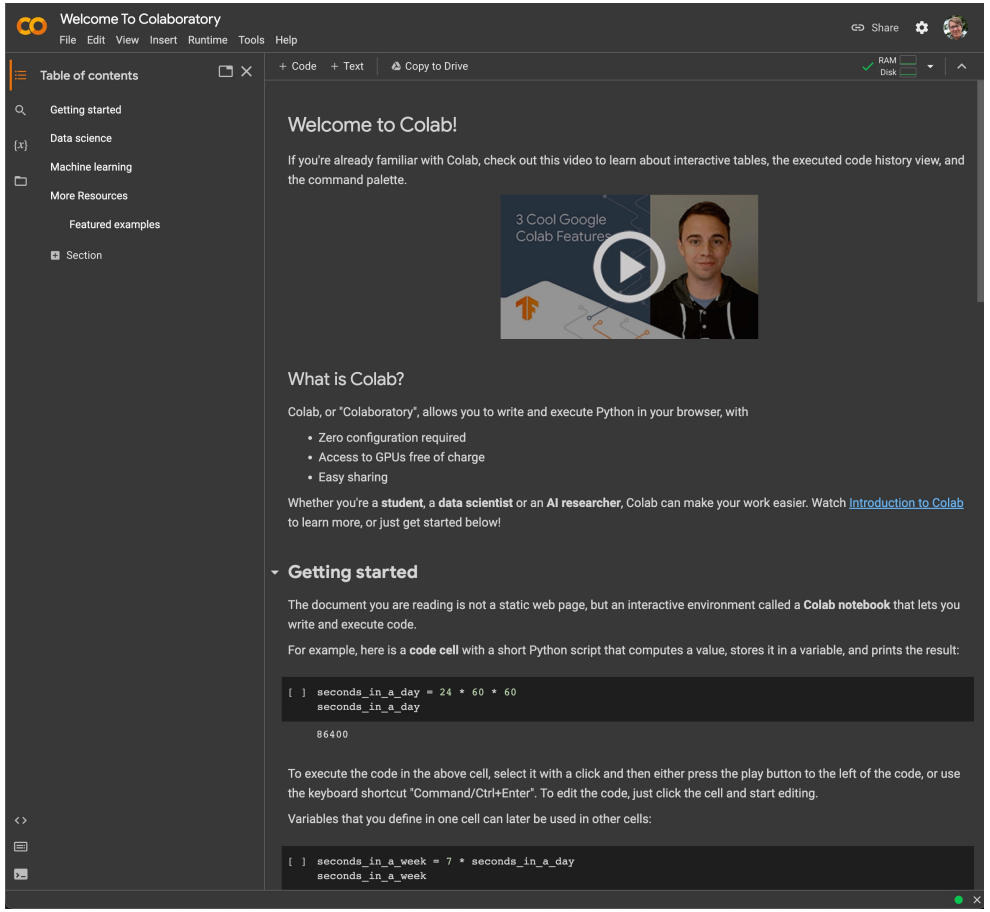
Cloud service

- Google Colab, Amazon Sagemaker
- JupyterHub (e.g., jhub.dartmouth.edu)

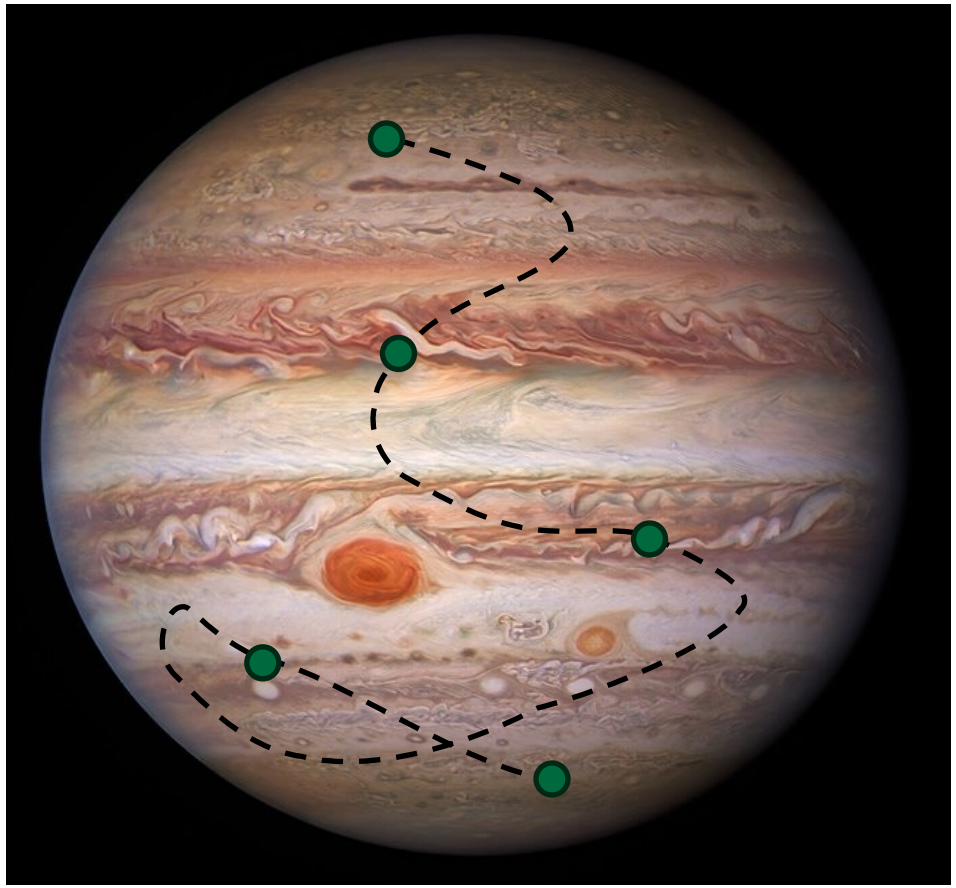


Source: https://colab.research.google.com/

A Walk around Jupyter: Hands-on

Itinerary

- General layout and interface elements
- Markdown cells
- Code cells
- Producing figures
- Magic commands

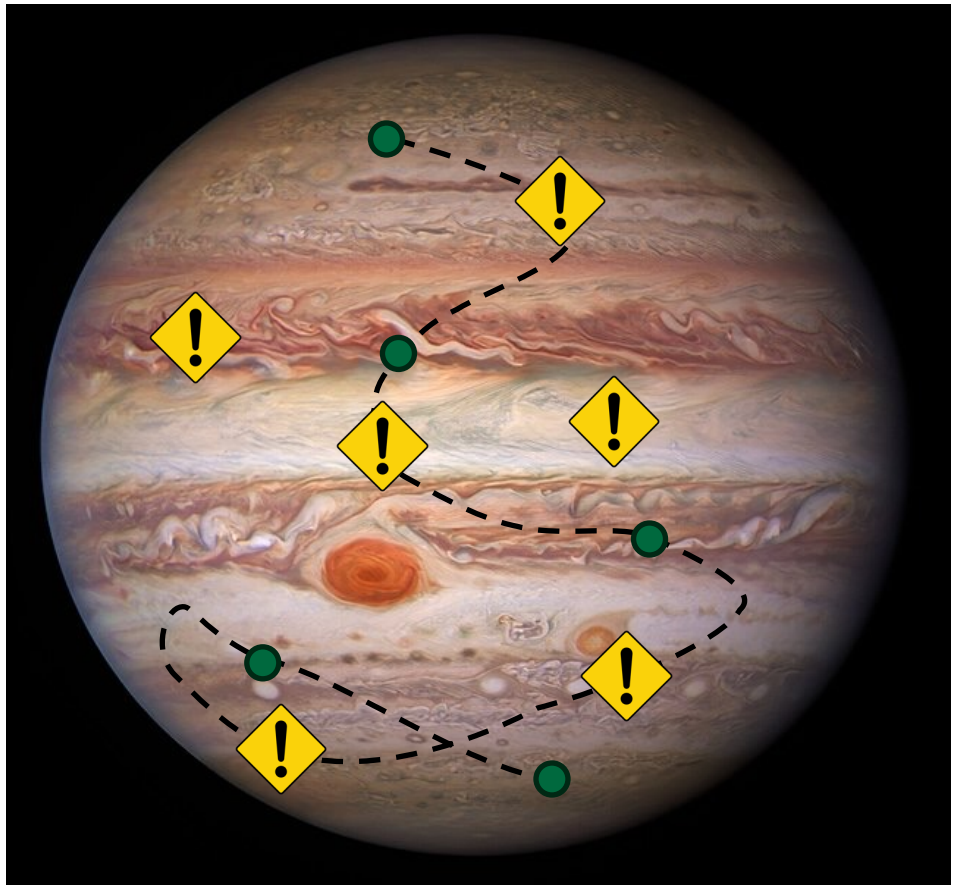


NASA/ESA/NOIRLab/NSF/AURA/M.H. Wong and I. de Pater (UC Berkeley) et al.Acknowledgments: M. Zamani, CC BY 4.0, via Wikimedia Commons

What to look out for

- Running code out of order
- “God notebooks”
- Discouraging modularity
- Difficulty to test and debug code
- Version control can be challenging
- Reproducibility may be an illusion:
  - Only 3 % of notebooks from scientific publications truly reproducible

Samuel, S., & Mietchen, D. (2023). Computational reproducibility of Jupyter notebooks from biomedical publications. *arXiv preprint arXiv:2308.07333*.



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When to use Jupyter Notebooks

🚀 Drafting, rapid prototyping

📊 Creating visualizations

Reporting

🎓 Education and Teaching

🔄 Stand-alone tasks that are not part of a bigger pipeline

♻️ When reusability of code is not a concern

Next steps

- Widgets:
  - Graphical user interface controls (sliders, checkboxes, text inputs, …)
- Nbconvert
  - Convert your notebook into a static format (PDF, HTML, LaTeX, Markdown, …)
- Voilà
  - Turn your notebook into a dashboard or web app

Questions

Thank you.