

Interactive Supercomputing with Jupyter Notebooks

Tutorial on Python for HPC

CSCS-USI Summer School 2019

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July 17, 2020

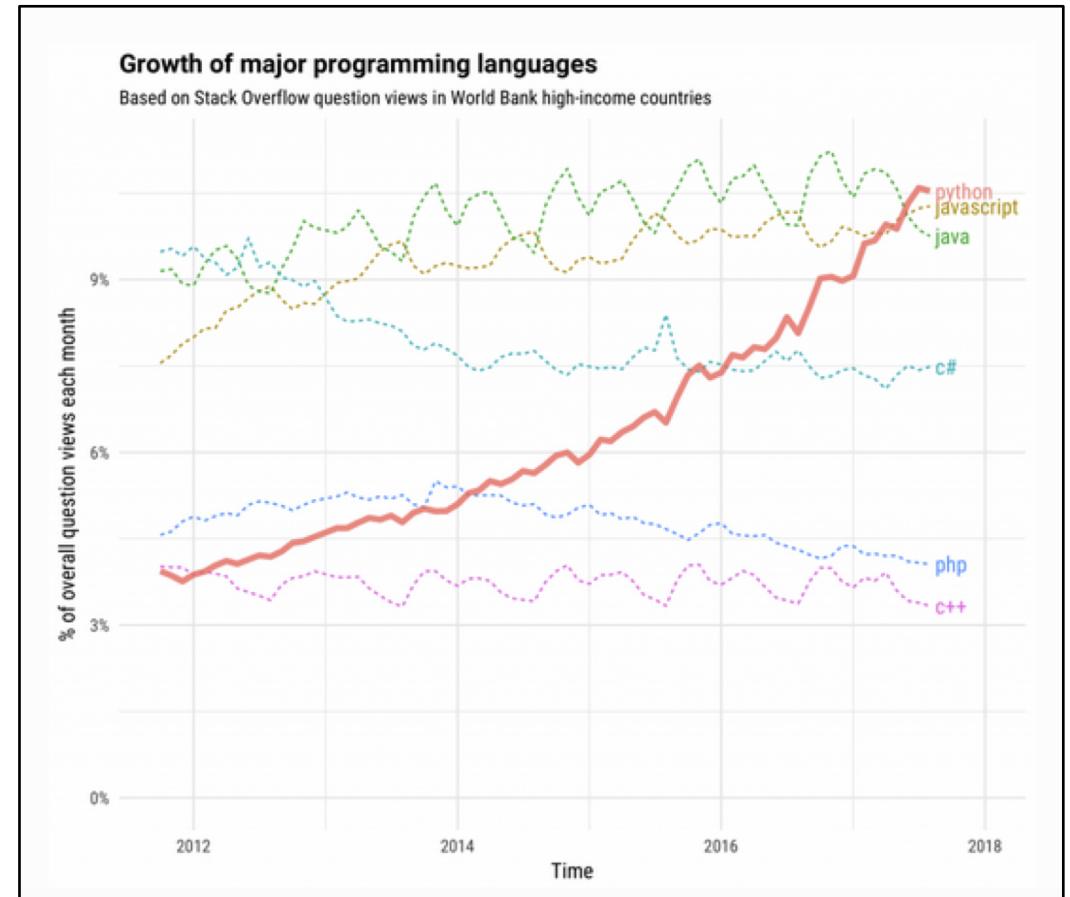
Schedule for today

- 09:00 – 10:45 Interactive Supercomputing with JupyterLab
- 10:45 – 11:00 Break
- 11:00 – 12:00 Python for HPC
- 12:00 – 13:00 Lunch
- 13:00 – 13:30 Networking (Spatial Chat)
- 13:30 – 15:30 Python for HPC (cont.)
- 15:30 – 16:00 Break
- 16:00 – 17:00 Q&A (Zoom)

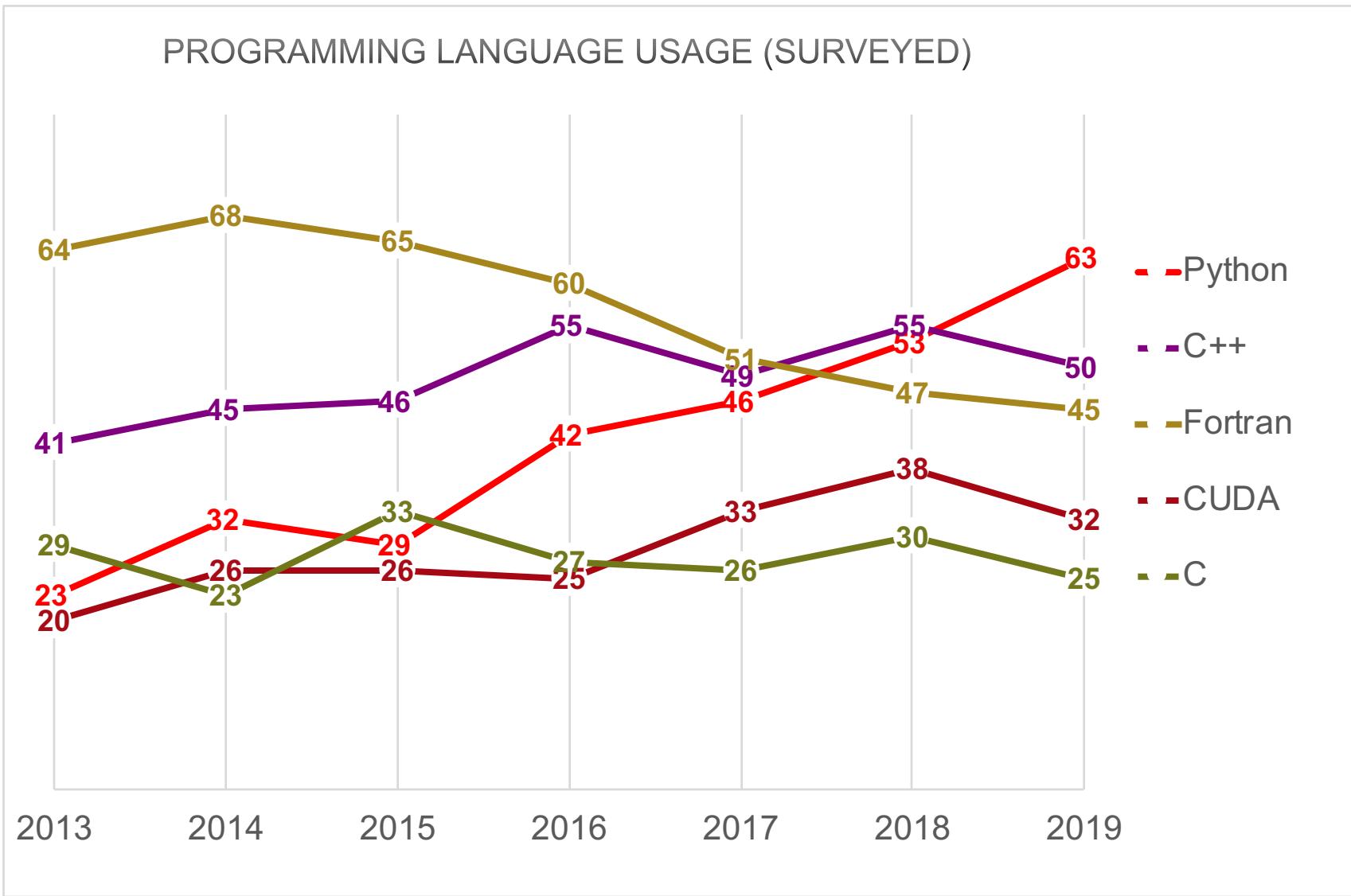
The rise of Python



- Python has grown to become a dominant language both in data analytics and general programming
- Rise fueled by computational libraries like Numpy, Pandas, and Scikit-Learn and libraries for visualization, interactive notebooks, collaboration, etc.
- Python long used as glue, for pre- and/or post-processing.. but increasingly used for simulation as well

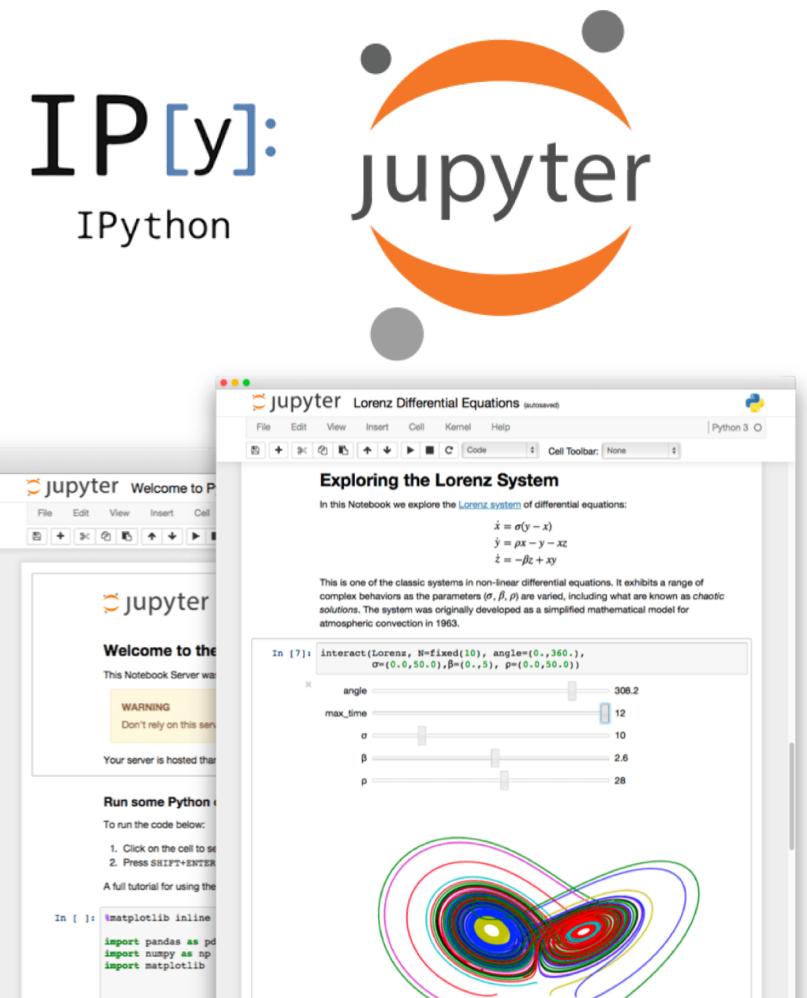


Python usage at CSCS



Jupyter Notebook

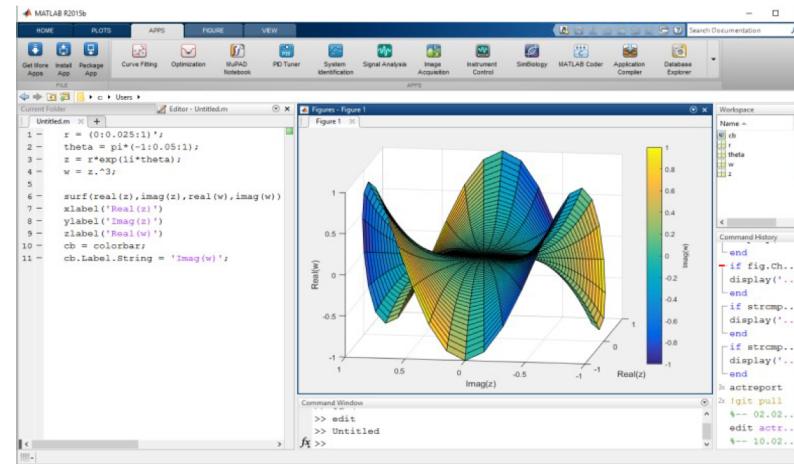
- Project Jupyter – reproducible **computational narratives**
- Mainly known for the Jupyter Notebook server
 - Web server and web app to **create documents that contain narrative text, equations, code, results, visualizations, and rich media**
- Attached to a “kernel”, which does the computation
- The document itself is also called a Jupyter Notebook (.ipynb, JSON format)
 - Easily shared with others
 - Can convert to PDF, HTML, LaTeX, ...
- The working environment includes
 - In-browser terminal
 - File browsing
 - Support for many languages: Python, R, Julia, C++, ...
 - Extensible design
 - Many server/client plugins
- Default implementation (IPython)



JupyterLab

- Next-generation web-based user interface for Jupyter
- Provides higher degree of interaction between notebooks, documents, text editors and other activities (arrange with tabs/splitters)
- Advanced interactive development environment
- Served from same server and uses same notebook document format

The screenshot shows the JupyterLab interface. On the left, there's a sidebar with 'File', 'Edit', 'View', 'Run', 'Kernel', 'Tabs', 'Settings', and 'Help'. Below it are sections for 'Notebooks' (with files like Data.ipynb, Fasta.ipynb, Julia.ipynb, R.ipynb, iris.csv, lightning.json, lorenz.py), 'Running' (seconds.egg), 'Commands' (lorenz.ipynb), 'Cell Tools', and 'Tabs'. The main area has tabs for 'Lorenz.ipynb' (active), 'Terminal 1', 'Console 1', 'Data.ipynb', and 'README.md'. The 'Lorenz.ipynb' tab shows a text cell with the Lorenz equations and a code cell with parameters sigma=10.0, beta=2.67, rho=28.0, and a resulting 3D plot of the Lorenz attractor.



JupyterLab Extensions

- JupyterLab is designed as a customizable, extensible environment
- Extensions can provide new themes, file viewers and editors, and renderers for rich output
- 100 GitHub repos tagged “jupyterlab-extensions”
- Examples include:
 - Memory usage
 - Dask dashboard
 - Tensorboard
 - GPU dashboards





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Sharing notebooks

Sharing static notebooks

<https://nbviewer.jupyter.org/>

nbviewer

A simple way to share Jupyter Notebooks

Enter the location of a Jupyter Notebook to have it rendered here:

URL | GitHub username | GitHub username/repo | Gist ID

Go!

Programming Languages

IPython



IRuby



IJulia

An IJulia Preview

This notebook is a preview demo of IJulia: a [Julia language](#) backend combined with the [IPython](#) interactive environment. This combination allows you to interact with the Julia language using IPython's powerful [graphical notebook](#), which combines code, formatted text, math, and multimedia in a single document.



• Note: this is a preview, because it relies on pre-release bleeding-edge versions of Julia, IPython, and several Julia packages, as explained on the [Julia GitHub page](#), and functionality is evolving rapidly. We hope to have a more polished release soon.

Basic Julia interaction

Sharing live notebooks

<https://mybinder.org/>



Turn a Git repo into a collection of interactive notebooks

Have a repository full of Jupyter notebooks? With Binder, open those notebooks in an executable environment, making your code immediately reproducible by anyone, anywhere.

Build and launch a repository

GitHub repository name or URL

GitHub repository name or URL

GitHub ▾

Git branch, tag, or commit

Git branch, tag, or commit

Path to a notebook file (optional)

Path to a notebook file (optional)

File ▾

launch

Copy the URL below and share your Binder with others:

Fill in the fields to see a URL for sharing your Binder.

Copy the text below, then paste into your README to show a binder badge:

launch binder



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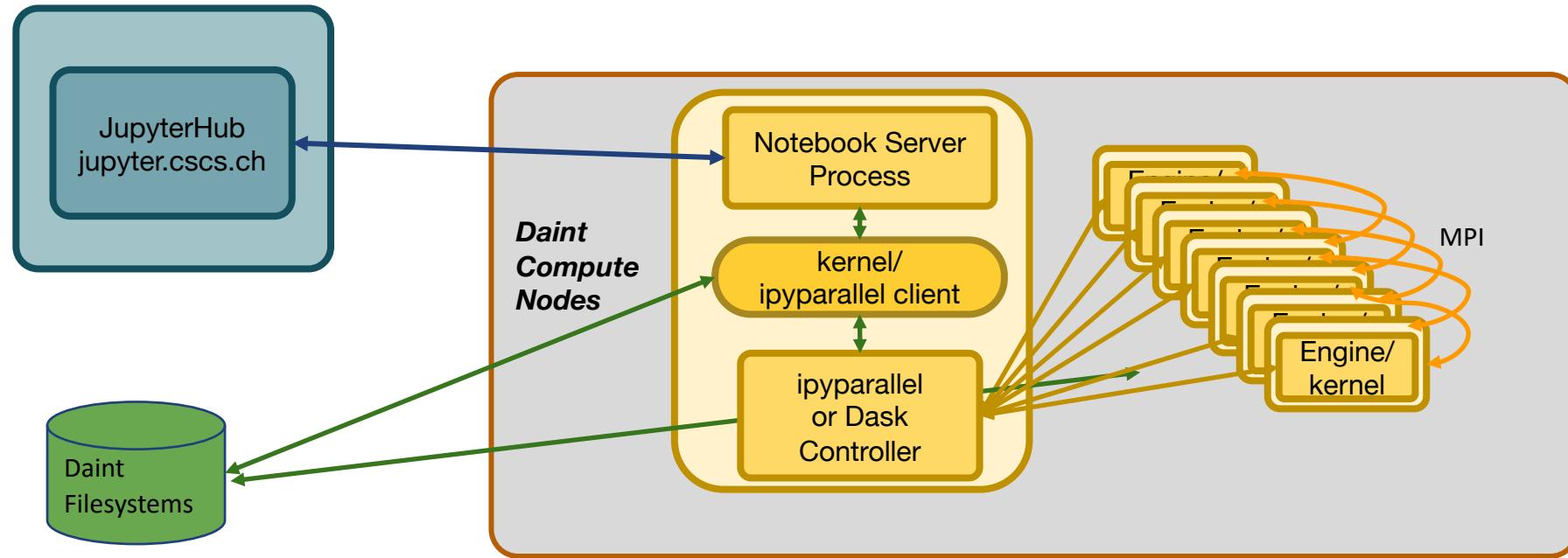
JupyterHub

JupyterHub

- JupyterHub is a way to give Jupyter notebook servers to a group of users – e.g. users of a supercomputing site, a research group, a [virtual!] classroom of summer school students, ...



JupyterHub on Piz Daint



JupyterHub at CSCS

The screenshot shows a web browser window for the URL <https://jupyter.cscs.ch>. The page title is "JupyterHub". The header features the CSCS logo and the ETH Zürich logo. A large white box contains the "Sign in to access JupyterLab" form. The form has two input fields: "Username" and "Password", both with placeholder text. Below the fields is a red "SIGN IN" button. At the bottom of the form are links for "Help", "Privacy", and "Terms". The footer contains the text "Swiss National Supercomputing Centre" and "Via Trevano 131, 6900 Lugano, Switzerland", along with a phone number "+41 91 610 08 11" and an email address "Email - help@cscs.ch". Social media icons for Twitter, YouTube, Facebook, and LinkedIn are also present.

The screenshot shows a web browser window for the URL <https://jupyter.cscs.ch>. The page title is "JupyterHub". The header features the CSCS logo and the ETH Zürich logo. The user "robinson" is logged in, as indicated by the "User: robinson" dropdown. The main content area has tabs for "Home", "Token", and "Admin". Under the "Admin" tab, there is a configuration form for launching a JupyterLab instance. It includes dropdown menus for "Node Type" (set to "GPU"), "Nodes" (set to 1), and "Duration (hr)" (set to 1). A red "Launch JupyterLab" button is prominently displayed. The footer contains links for "Help", "Privacy", and "Terms", and the copyright notice "2019 © CSCS | www.cscs.ch".



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Demo of JupyterLab interface



Let's get going...

Please open a browser (**Firefox** or **Chrome**, no guarantees for the others...) and visit...

<https://jupyter.cscs.ch>