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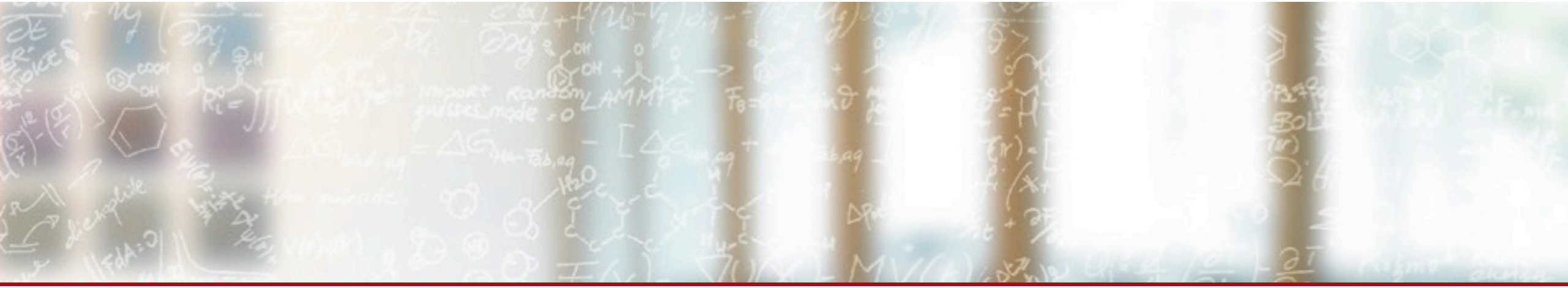

Interactive Computing with Jupyter on Piz Daint, using Python, ParaView and Julia

Tim Robinson, Jean Favre and Harmen Stoppels, CSCS

Apr 26, 2021

Agenda

09:00 – 10:45	**Jupyter, JupyterLab and JupyterHub on Piz Daint**
10:45 – 11:00	*Break*
11:00 – 12:00	**ParaView and Jupyter, Part I**
12:00 – 13:00	*Lunch*
13:00 – 14:00	**ParaView and Jupyter, Part II**
14:00 – 14:15	*Break*
14:15 – 16:15	**Programming in Julia**

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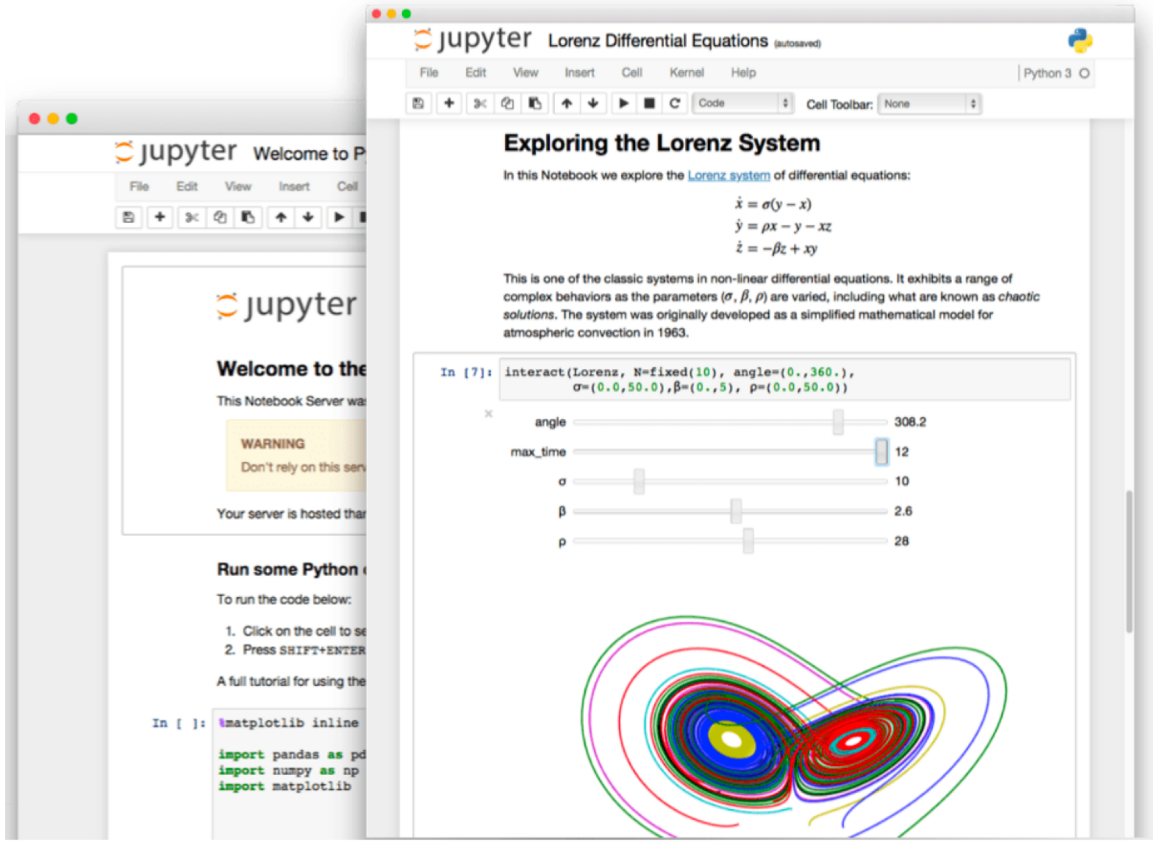
Part I: Jupyter: Jupyter Notebook, JupyterLab and JupyterHub

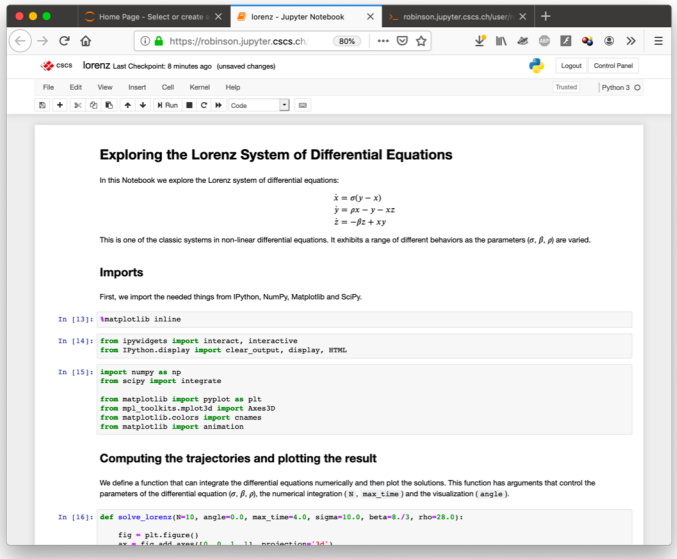
Jupyter Notebook

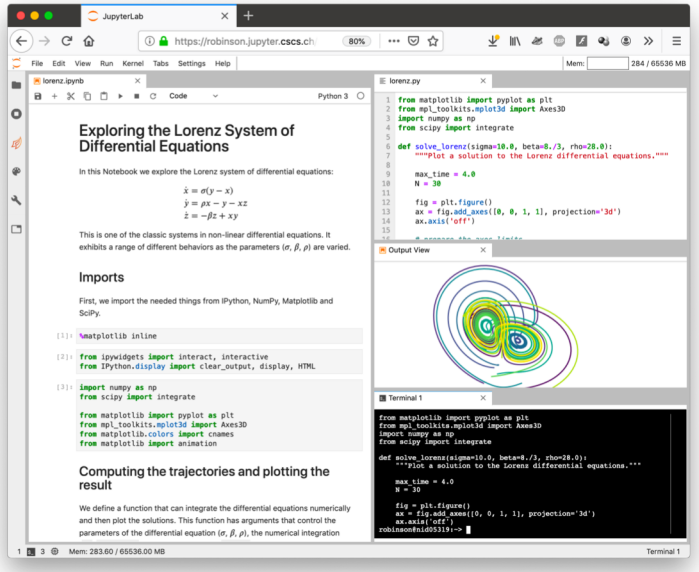
- Jupyter Notebook is an open-source web app for creating reproducible computational narratives
- Documents can contain live code, equations, narrative text, visualizations, and rich media
- Documents can be shared or exported to PDF, HTML, LaTeX, etc.
- Working environment includes
  - File browser
  - Terminal
  - Support for many languages: Python, R, Julia, C++, …
  - Extensible design
  - Many server/client plugins
- Notebook is attached to a “kernel”, which does the actual computation



JupyterLab

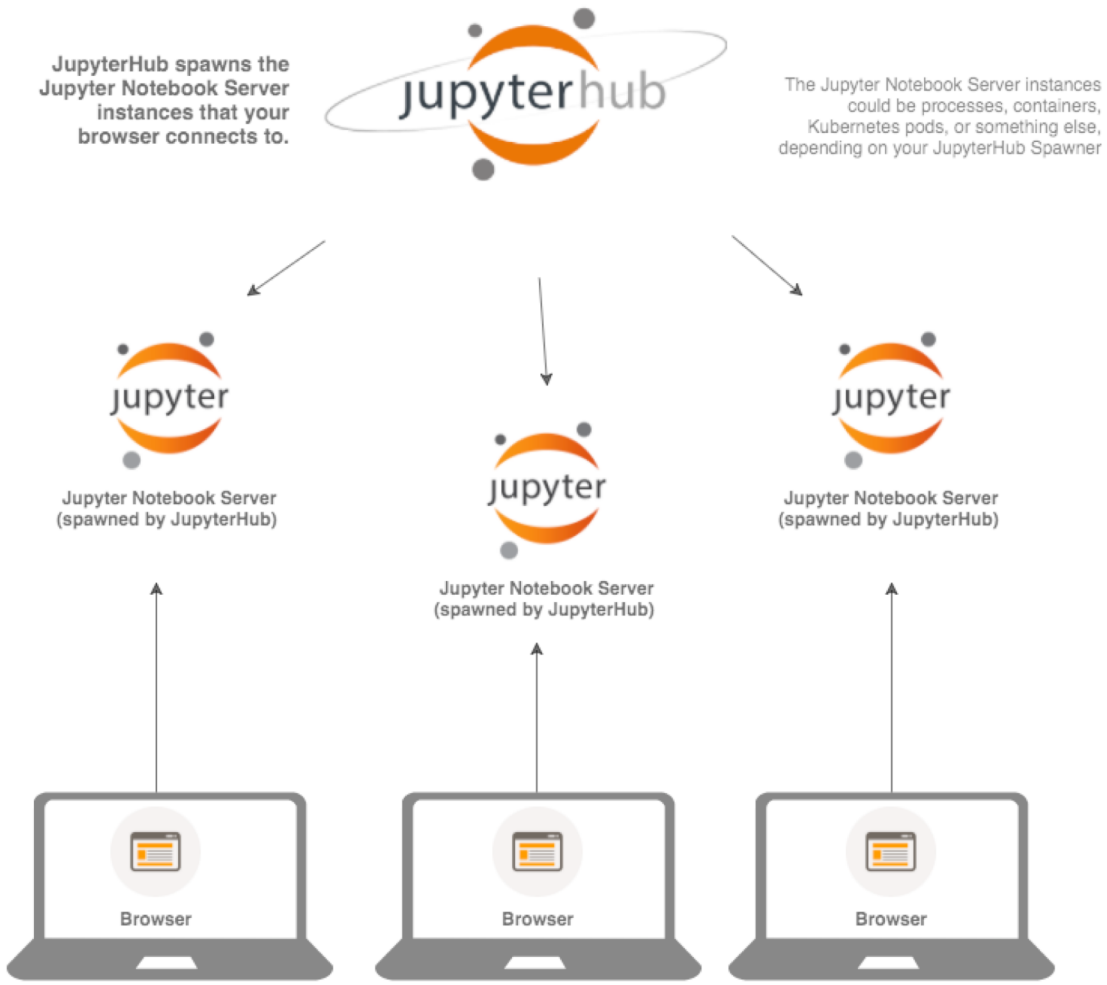
- JupyterLab is the next-generation user interface for Jupyter
- Higher degree of interaction between notebooks, documents, text editors and other activities (arrange with tabs/splitters)
- More advanced interactive development environment
- Uses the same notebook document format
- JupyterLab is the default interface at CSCS
- Classic notebook interface is still accessible by modifying the URL from /lab to /tree
  - Or: Help -> Launch Classic Notebook





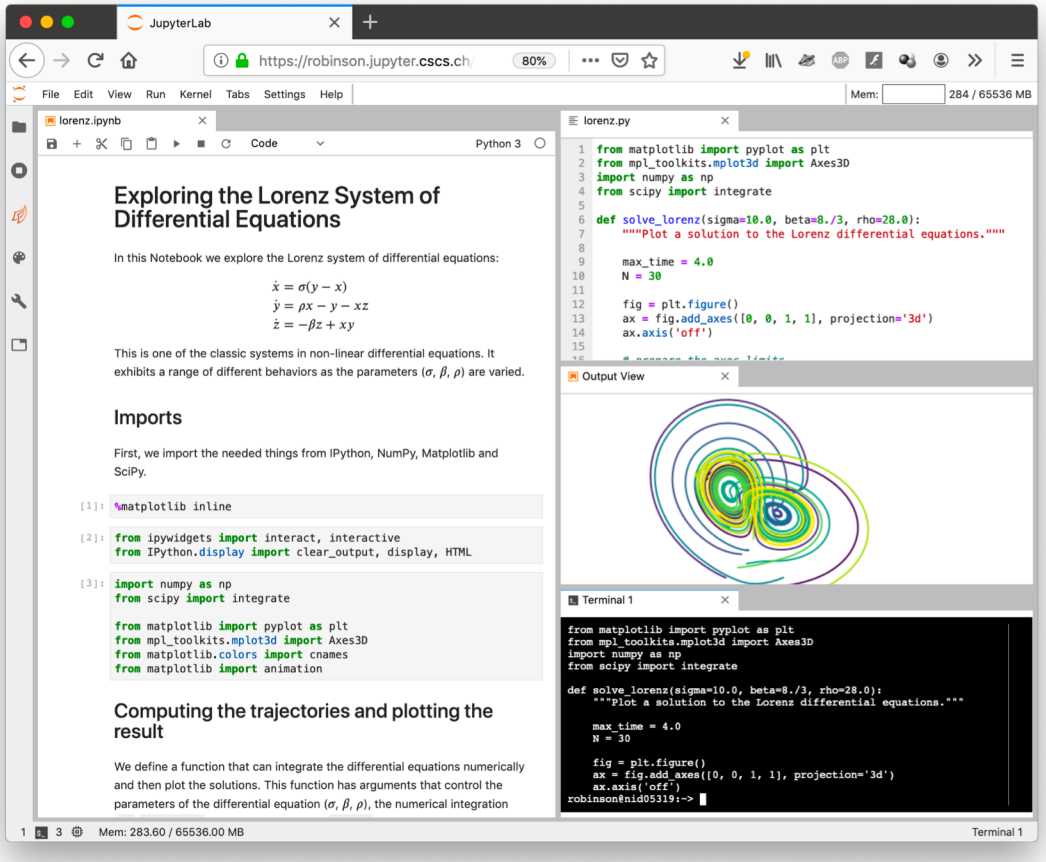
JupyterHub

- Multi-user server for Jupyter Notebooks (designed for classrooms, research labs, Universities...)
- Spawns, manages and proxies multiple instances of the single-user Jupyter Notebook server
- Main components:
  - **Hub** (tornado process)
  - **configurable http proxy** (node-http-proxy) that receives the requests from the client's browser
  - multiple **single-user Jupyter notebook servers** (Python/IPython/tornado) that are monitored by Spawners
  - an **authentication class** that manages how users can access the system

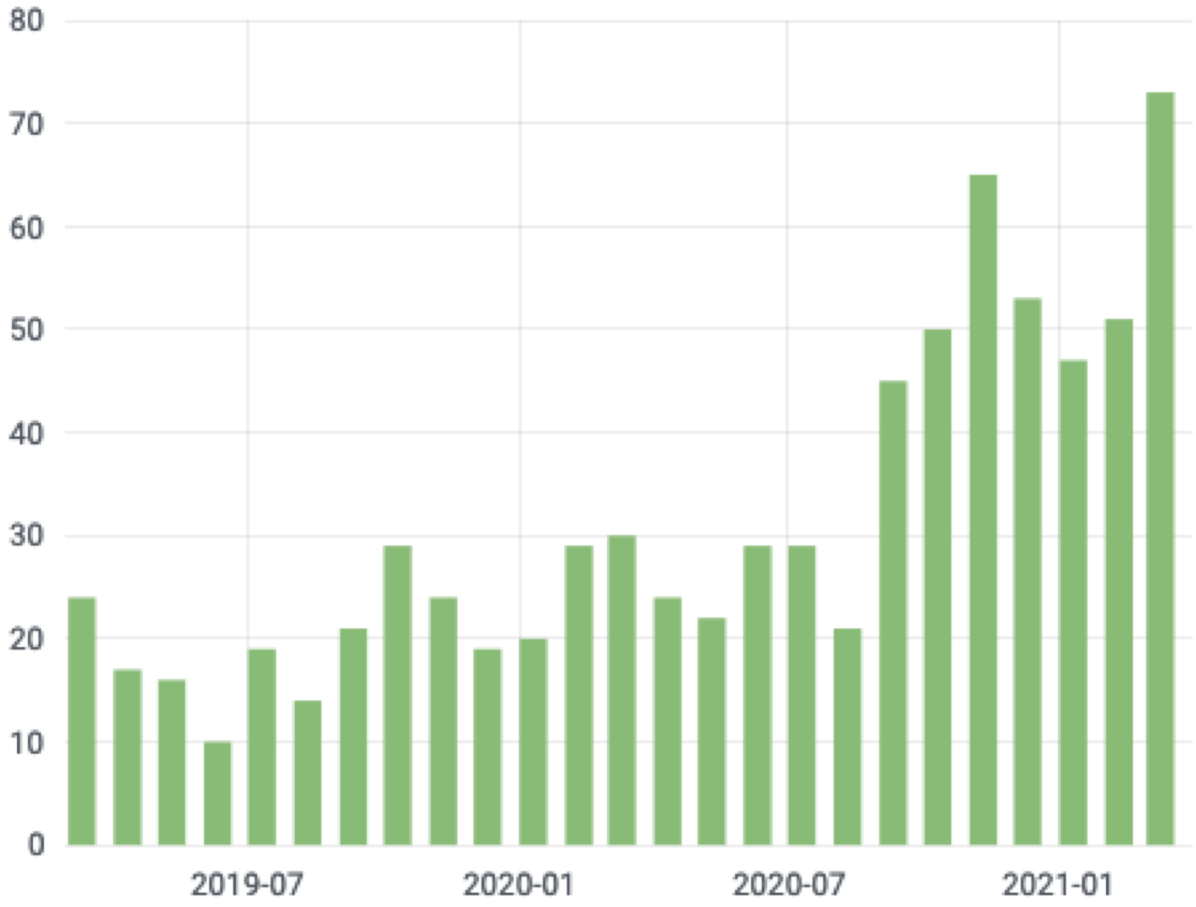


JupyterHub for Piz Daint

- JupyterHub for Piz Daint is accessible at:
  https://jupyter.cscs.ch
- Available to anyone with a compute allocation on Piz Daint
- Servers are launched on the compute nodes (GPU or multicore)
- You have dedicated access to the full compute capability of the node(s)
- Special Slurm reservations for interactive computing grow and shrink automatically according to demand
- In most cases you should have to wait less than five minutes for your allocation



JupyterHub monthly users on Piz Daint



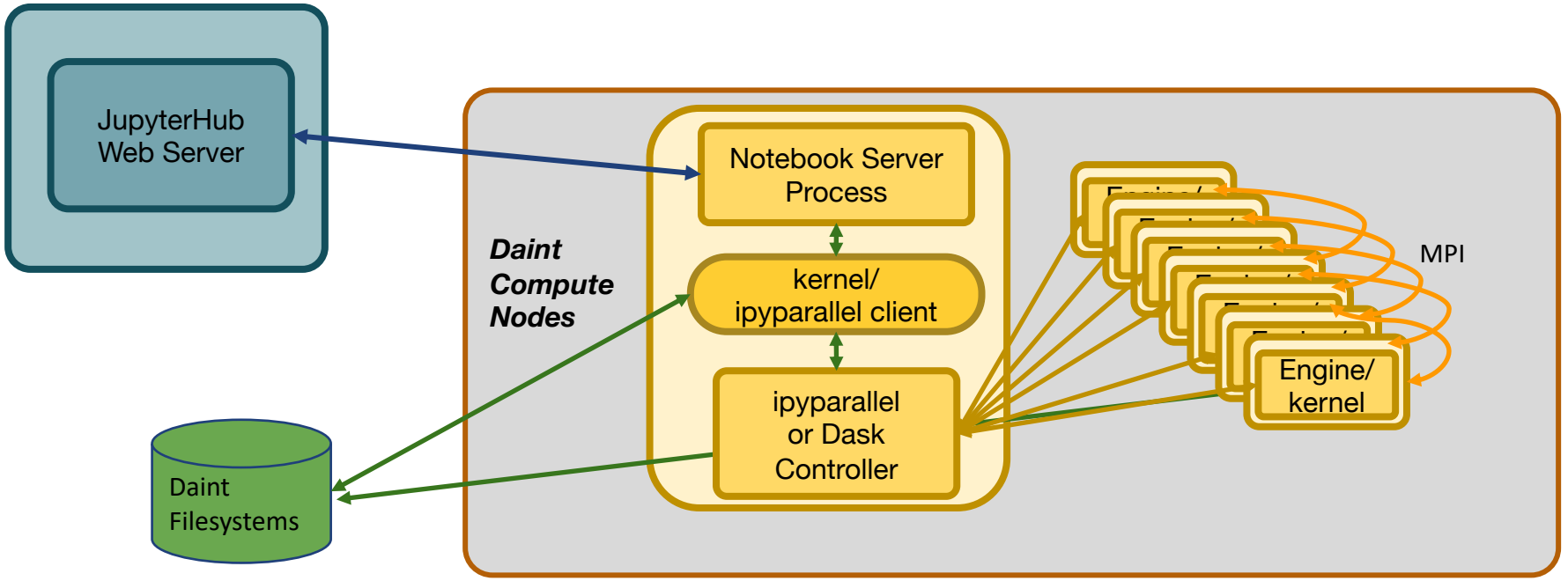
Challenges with interactive computing on HPC

- Shared parallel filesystems
- Network connectivity
- Slurm
- Warm swapping
- All kinds of other possible issues - usually these are temporal!

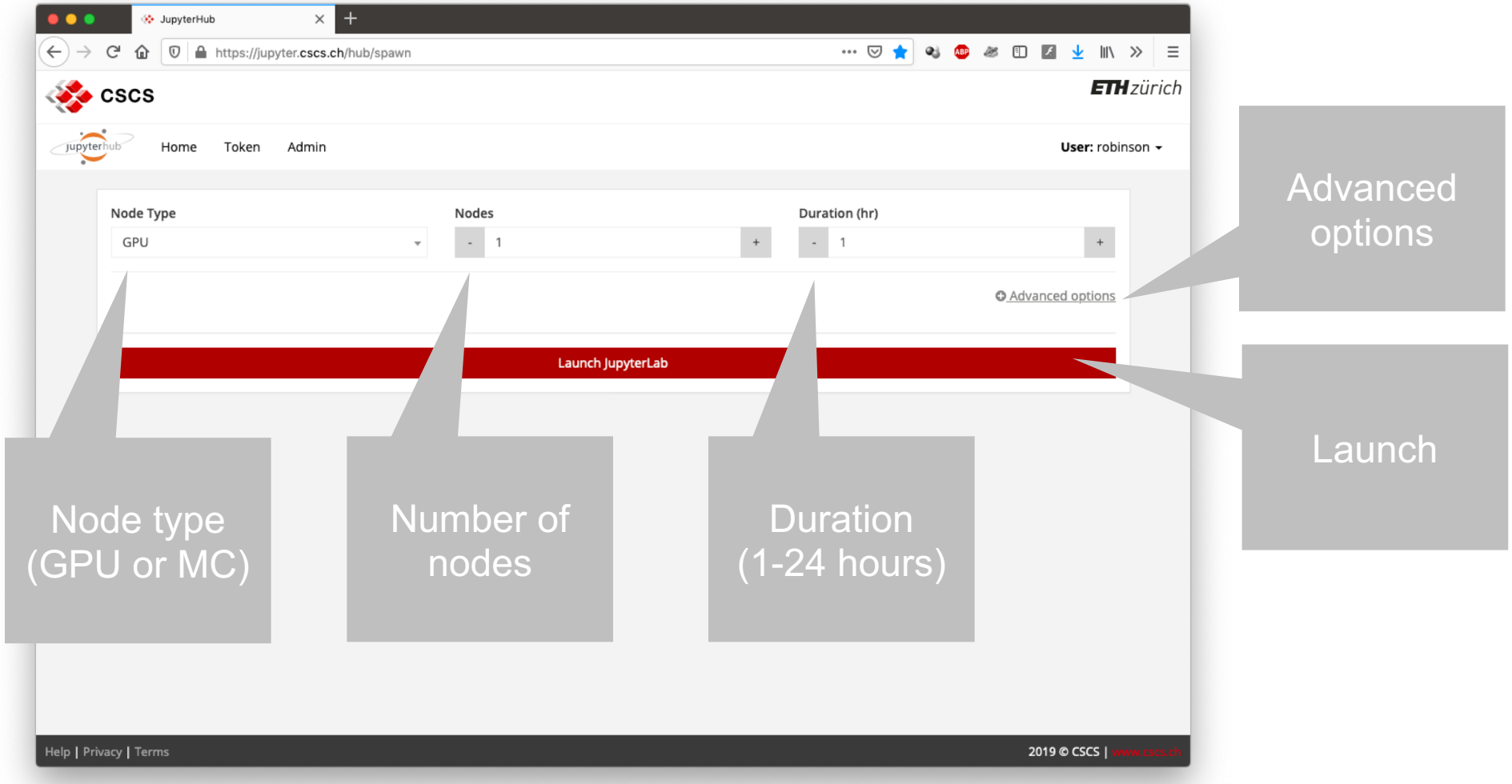
- Debugging problems:
  - Check for any maintenance announcements on the spawner page
  - Check your own internet connectivity
  - Check for old JupyterHub sessions in browser tabs (especially if kernels are not starting or are slow to connect or restart)
  - Inspect the Jupyter log file in your $SCRATCH directory
  - If problems persist, submit a ticket at https://support.cscs.ch
    - Include as much detailed information as possible – precise time periods, Slurm jobid, what was working, what was not working...

JupyterHub implementation at CSCS

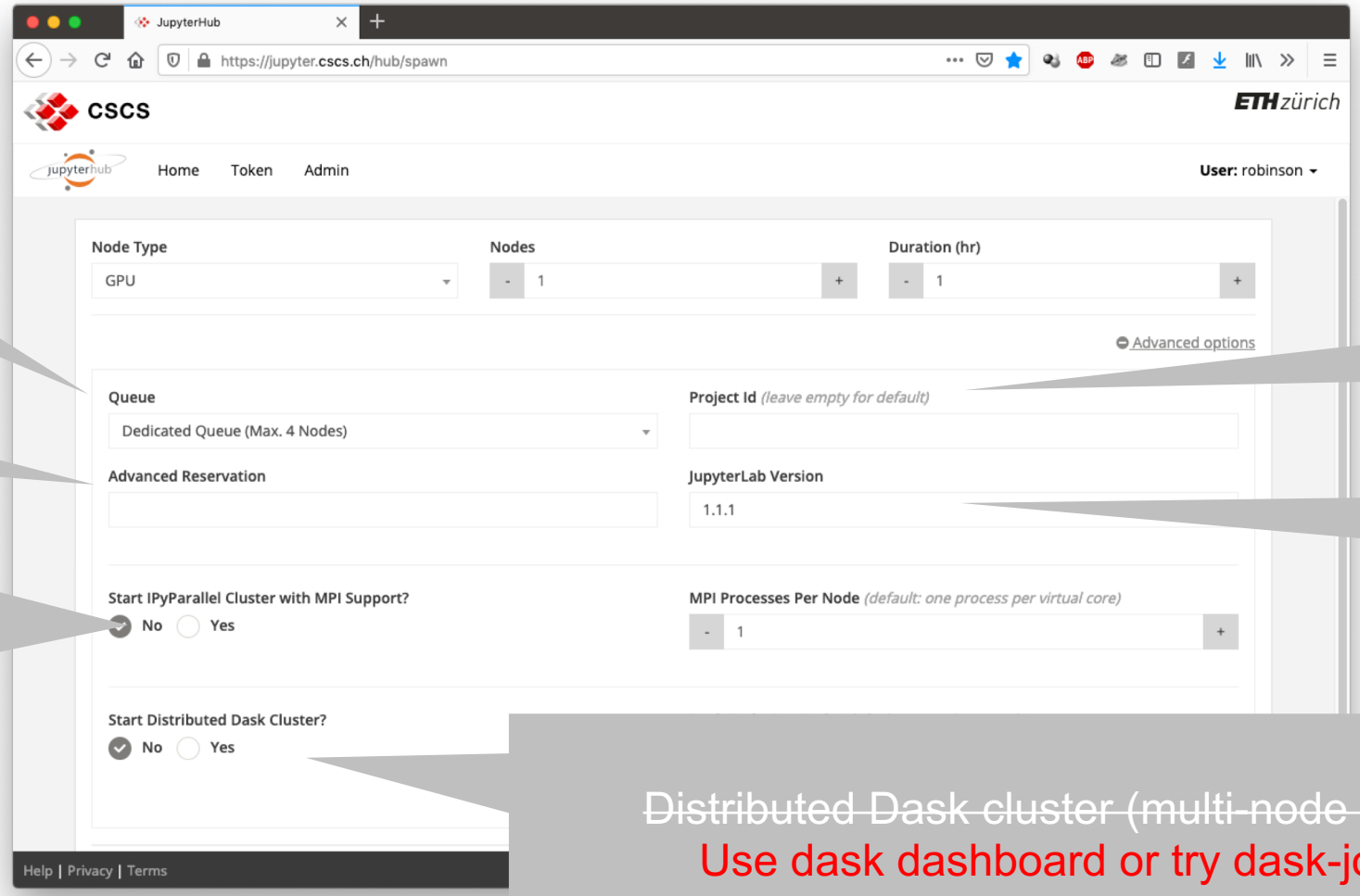
jupyter.cscs.ch



Basic options



Advanced options



Queue

Reservation

~~IPyParallel (multi-node notebooks)~~
Replaced by ipcluster magic

Project Id (account)

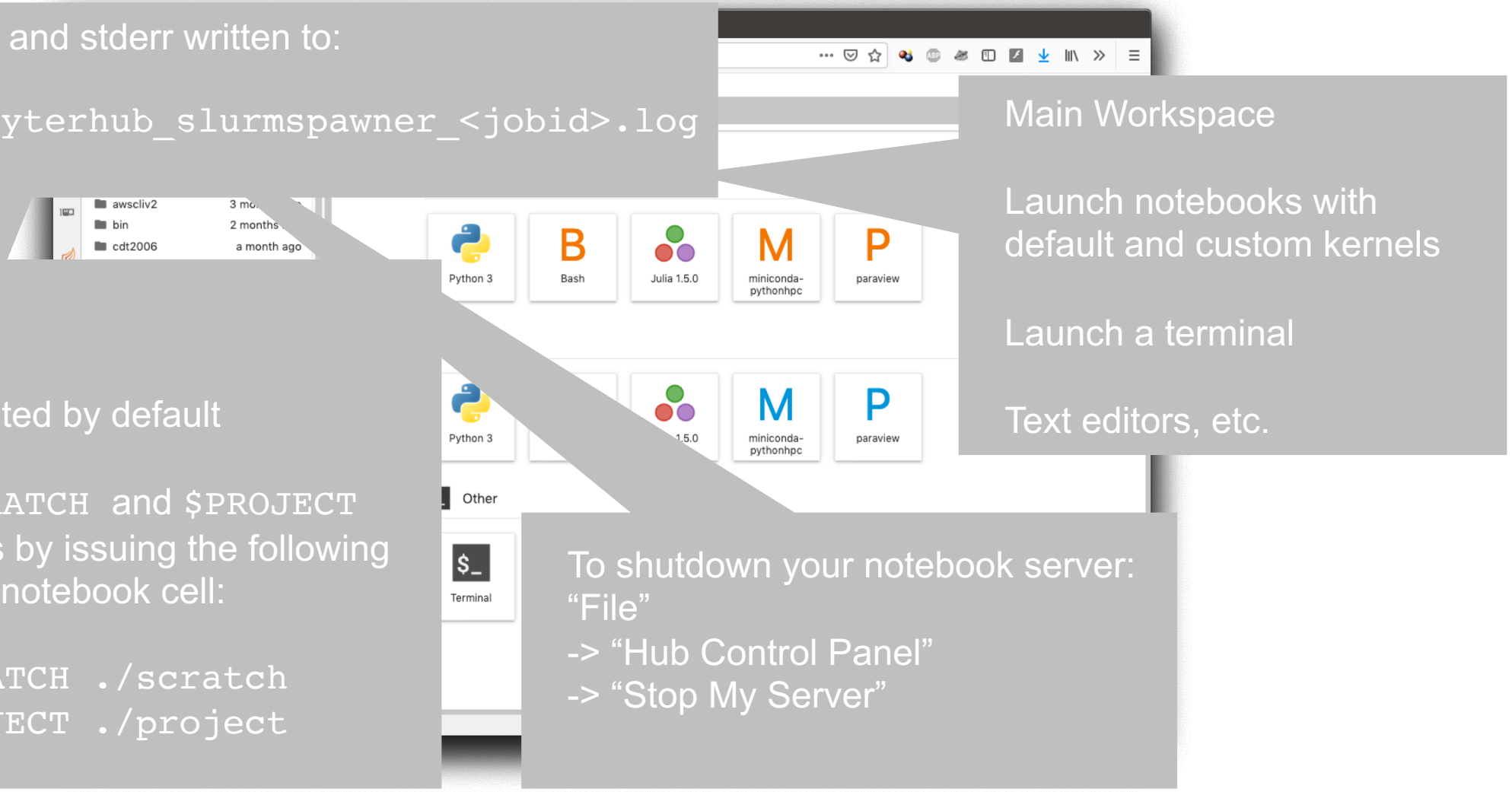
JupyterLab version

~~Distributed Dask cluster (multi-node notebooks)~~
Use dask dashboard or try dask-jobqueue

JupyterLab interface

Standard output and stderr written to:

`$SCRATCH/jupyterhub_slurmspawner_<jobid>.log`



File Browser

`$HOME` is mounted by default

To access `$SCRATCH` and `$PROJECT` create sym links by issuing the following commands in a notebook cell:

```
!ln -s $SCRATCH ./scratch
!ln -s $PROJECT ./project
```

Main Workspace

Launch notebooks with default and custom kernels

Launch a terminal

Text editors, etc.

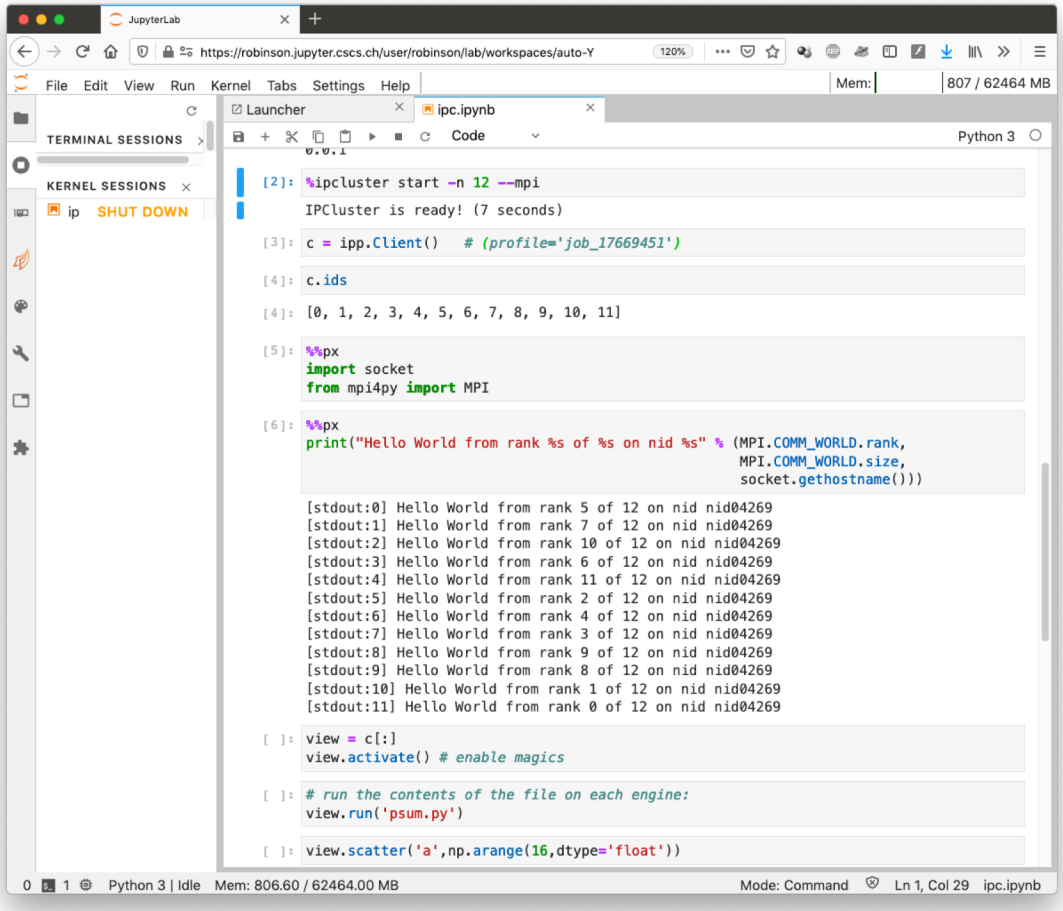
To shutdown your notebook server:
“File”
-> “Hub Control Panel”
-> “Stop My Server”

Getting the Python packages you need

- **pip install**, direct from the notebook (simple)
- **Virtual environments and kernels** (better)
- **module load** commands in $HOME/.jupyterhub.env (can be useful)
- Install **miniconda** and use **conda** environments (if you prefer conda)
- **Containers** (work in progress; potentially offers more flexibility)

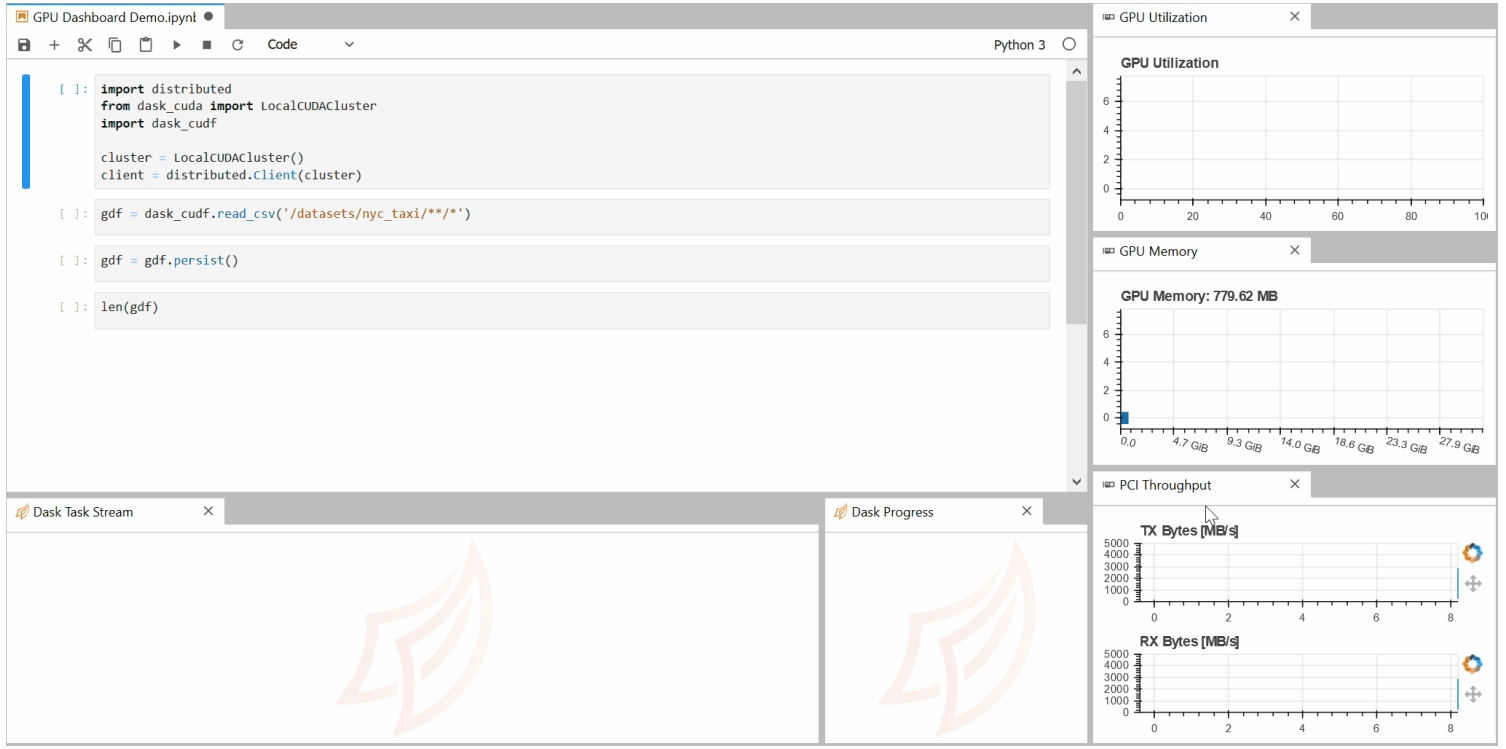
IPyParallel and ipcluster magic

- IPCluster magic commands for automatically starting and stopping ipyparallel clusters (ipcontroller and ipengines)
- `module load ipcmagic` in $HOME/.jupyterhub.env
- `import ipcmagic` in notebook
- Makes it easier to use MPI directly in the notebook

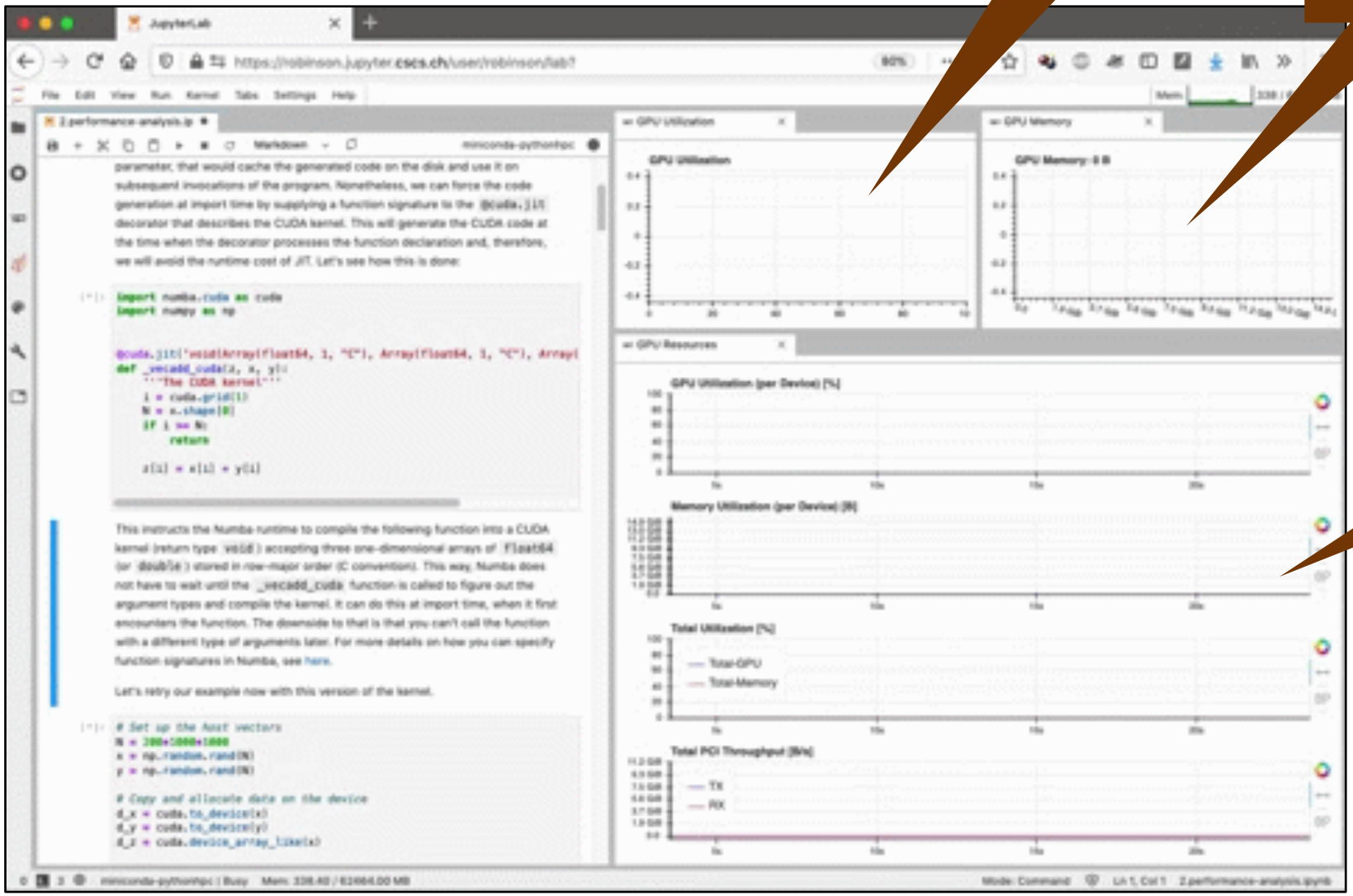


NVDashboard and Dask Distributed JupyterLab Extensions

- NVDashboard is a JupyterLab extension for displaying dashboards of GPU usage (from the NVIDIA RAPIDS team)
- Dask JupyterLab extension provides a way to manage Dask clusters, as well as embedding Dask's dashboard plots directly into JupyterLab panes



GPU dashboards



Let’s crack on…