JupyterHub at NCAR

and related things

Davide Del Vento

Computational & Information Systems Laboratory

NCAR
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

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Wednesday, September 23 2020

10am in Colorado (or somewhere in the world….)

About the speaker

- Davide Del Vento, Ph.D. helping users of NCAR's HPC infrastructure since 2008
- It's fine to interrupt with questions in context of what I am discussing

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https://www.linkedin.com/in/delvento/

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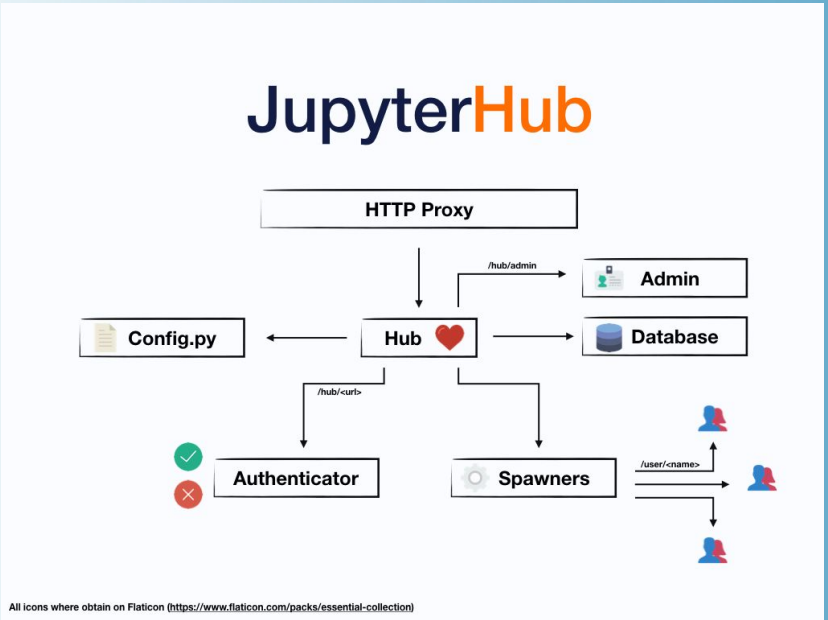
What is JupyterHub

- “The” way to serve Jupyter Notebooks to multiple users



Source: https://jupyterhub.readthedocs.io/en/stable/

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What is a Jupyter Notebook

- A single-user web app to create documents containing **arbitrary, user-provided live code**, equations, visualizations and narrative text

- Uses include: data cleaning and transformation, numerical simulation, statistical modeling, data visualization, machine learning, and much more

Source: https://jupyter.org/

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How this differs from old one

- The Jupyter (formerly ipython) Notebook has been available at NCAR since at least early 2015… and it still is...

- But requires a clumsy setup with double-login, ssh-tunneling, etc.
- Yet, that is more robust and so still supported

Doc: https://www2.cisl.ucar.edu/resources/jupyter-and-ipython

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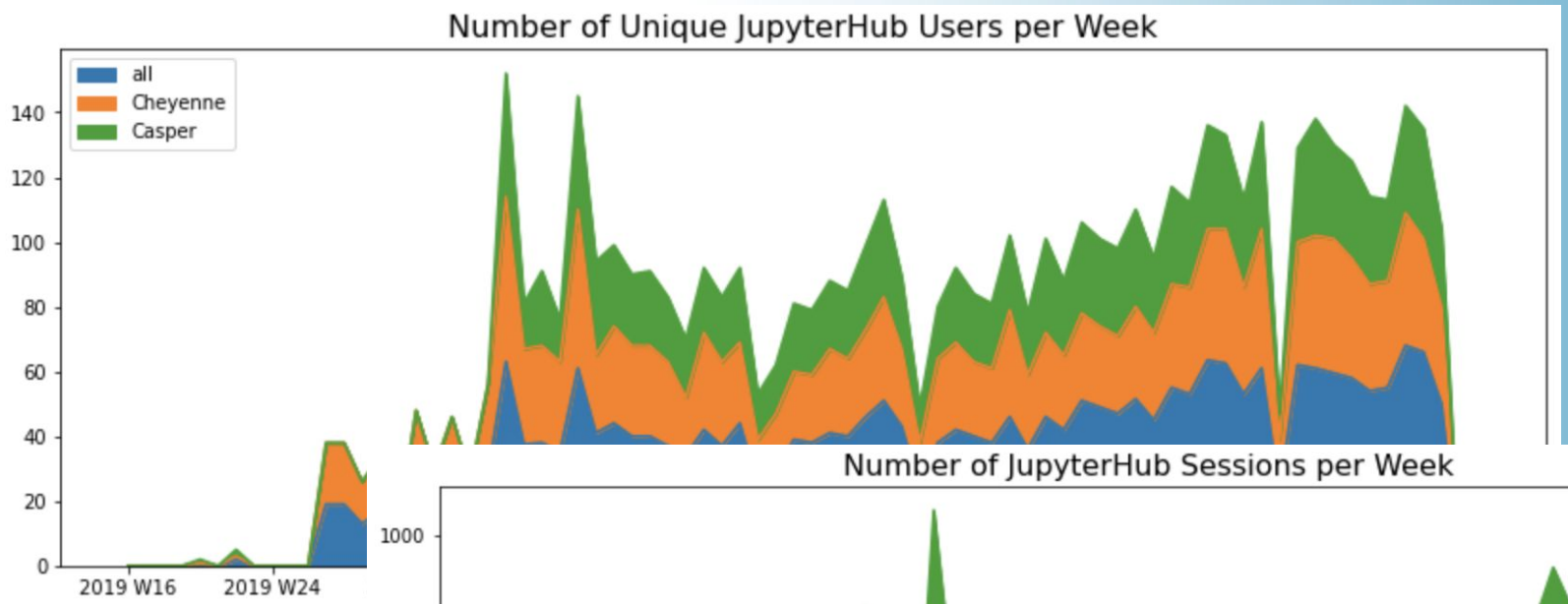

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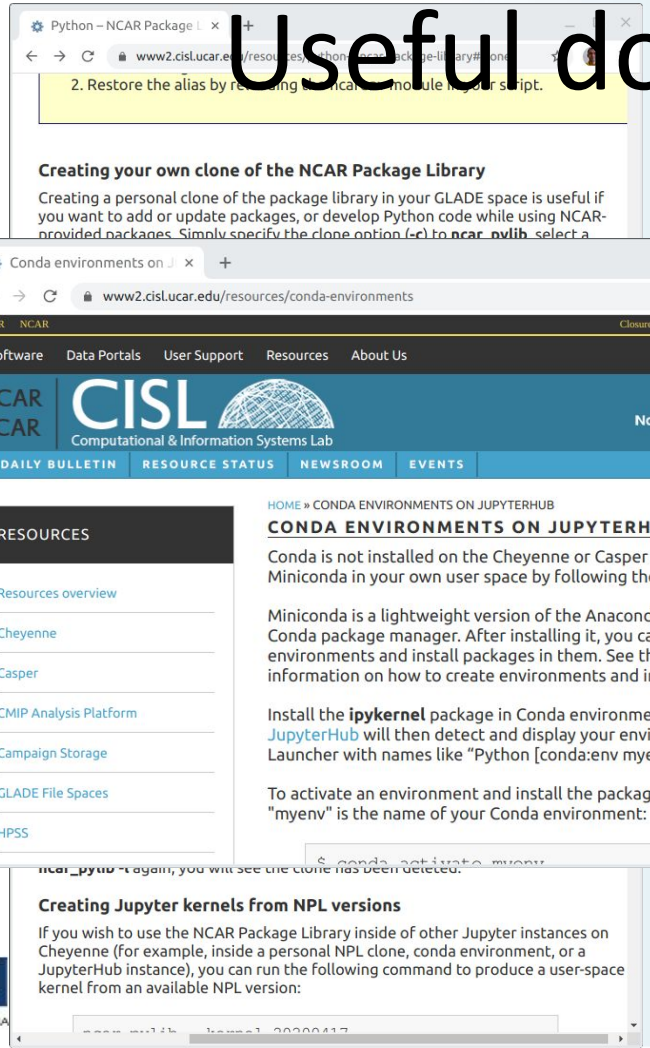
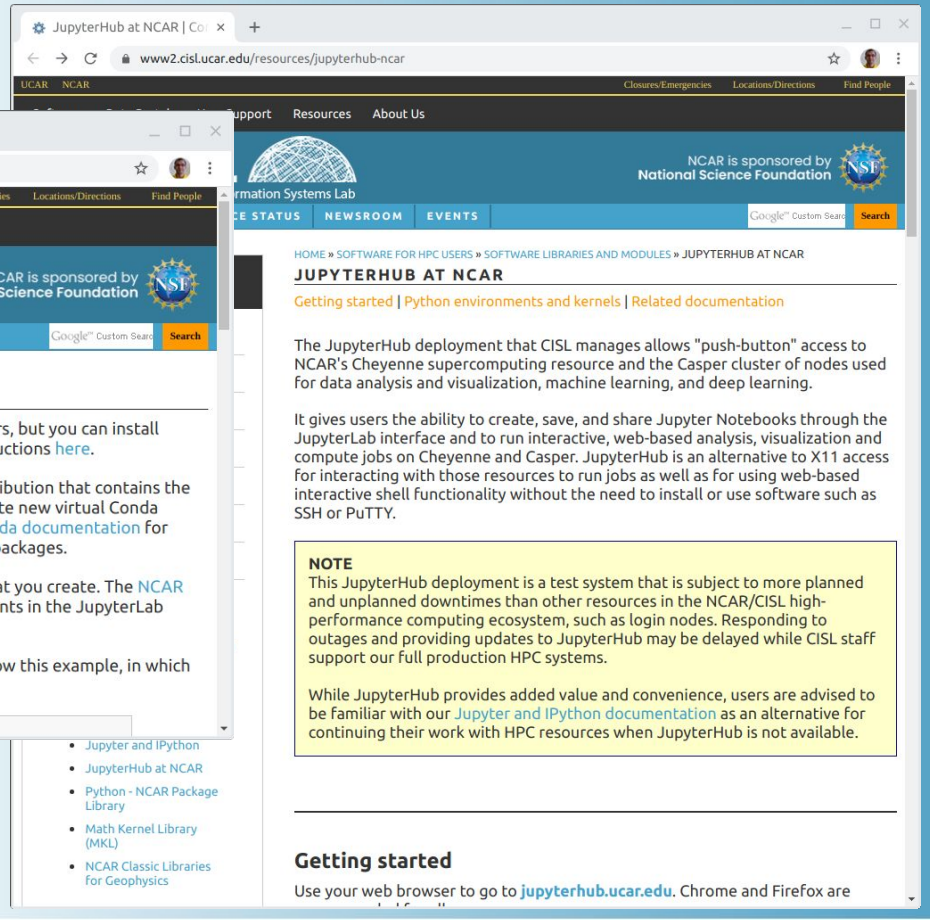
Useful documentation





Useful documentation

- https://www2.cisl.ucar.edu/resources/jupyterhub-ncar
- https://www2.cisl.ucar.edu/resources/python-%E2%80%93-ncar-package-library#clone
- https://www2.cisl.ucar.edu/resources/conda-environments
- https://www2.cisl.ucar.edu/resources/jupyter-and-ipython
- Stay tuned: more to come….

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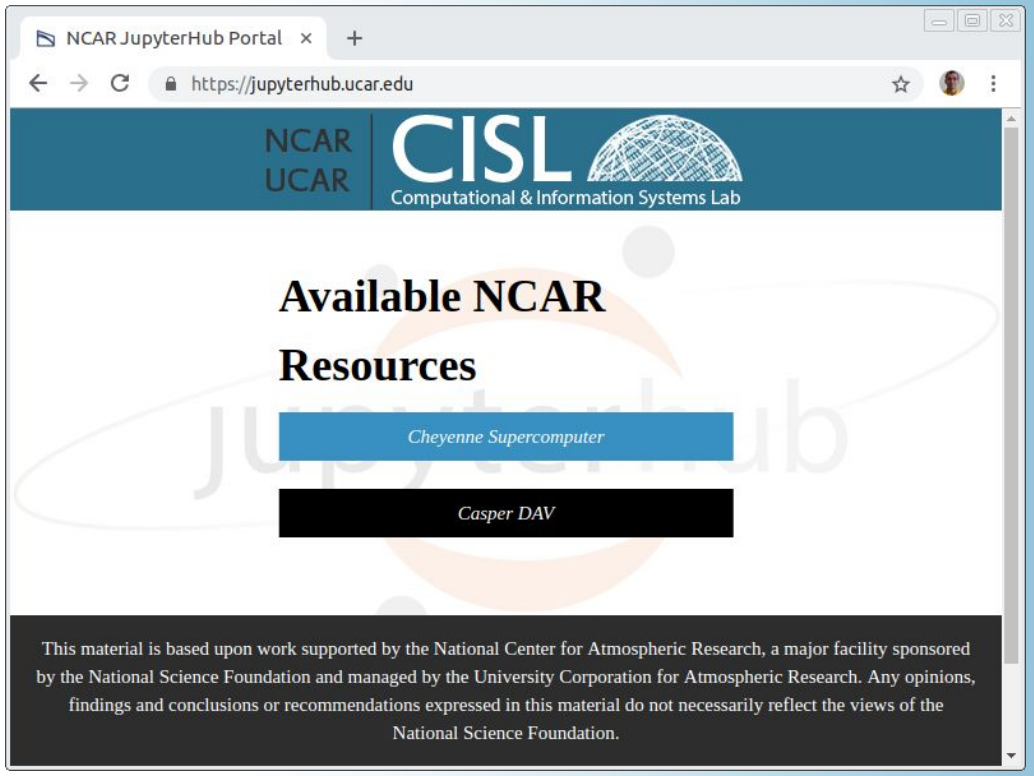
JupyterHub @ NCAR



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Demo or Backup slides

Where to go from here

- Documentation provides additional details
- Pangeo project provides specific information e.g. for parallel analysis
- Future talk will cover kernel customization

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CISL/NCAR documentation: see previous slides
Pangeo: http://pangeo.io/

Future work

- Ability to load modules before kernel startup
- Improve user-friendliness of the login process (e.g. kernel logos overlays)
- More documentation and training (let us know what you need!!)

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The end

- Thank you for your attention!
- Please fill a quick survey which will be sent to you
- Do not hesitate to contact user support
- Yes, slides and recording will be provided
- Any more questions?

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Backup slides

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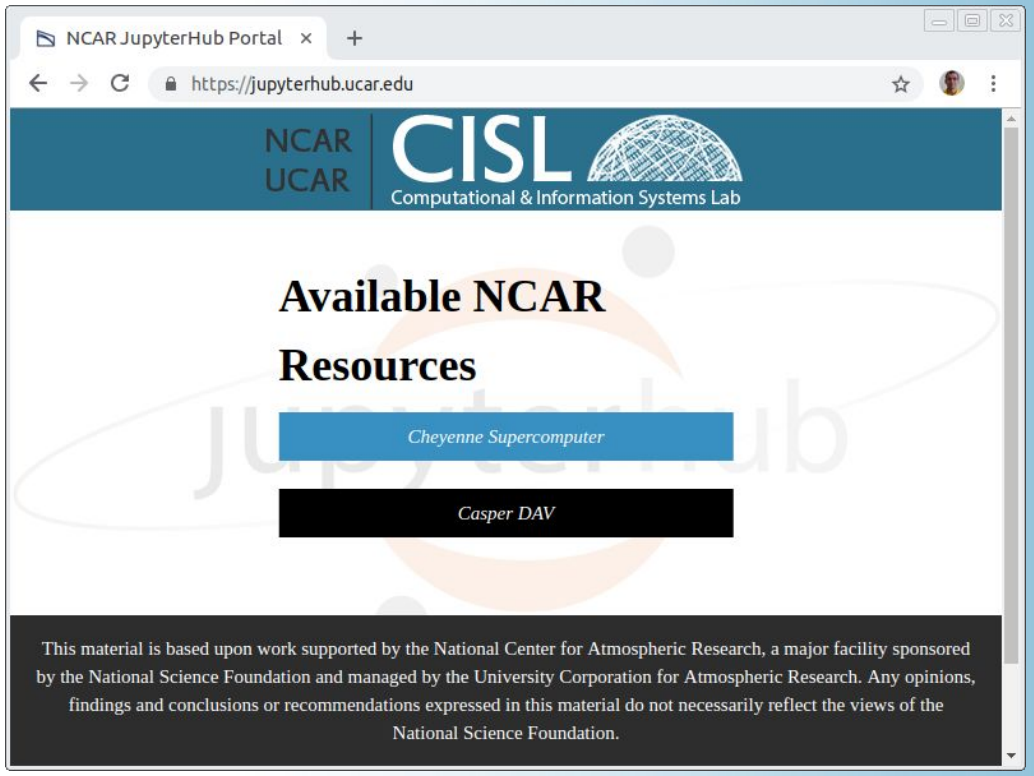
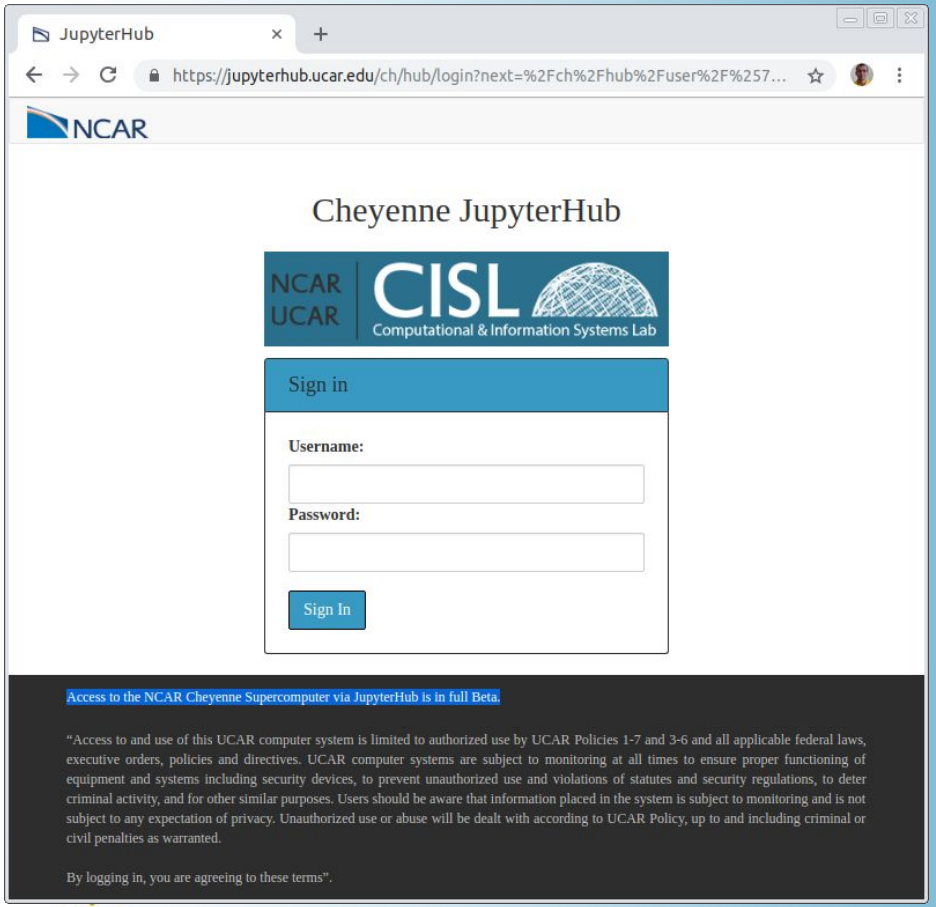
Logging in JupyterHub



Chrome & Firefox are recommended

Note the highlighted: this is beta



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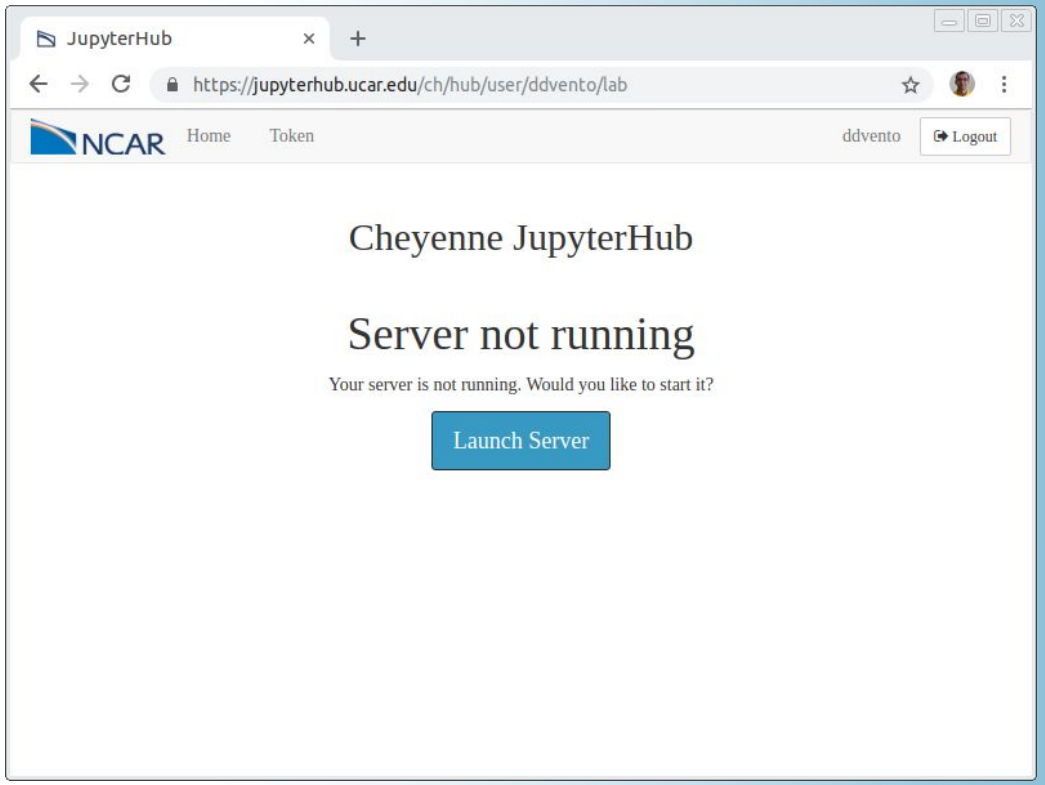
Starting the Jupyter Server



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What is a Jupyter Server?

- A program responding to HTTP requests
- For a single user!!!
- The same program you can start yourself “the old way” or on your laptop
- Usually “inaccessible” from the outside
- Needs “something” to become accessible (e.g. ssh-tunnel)

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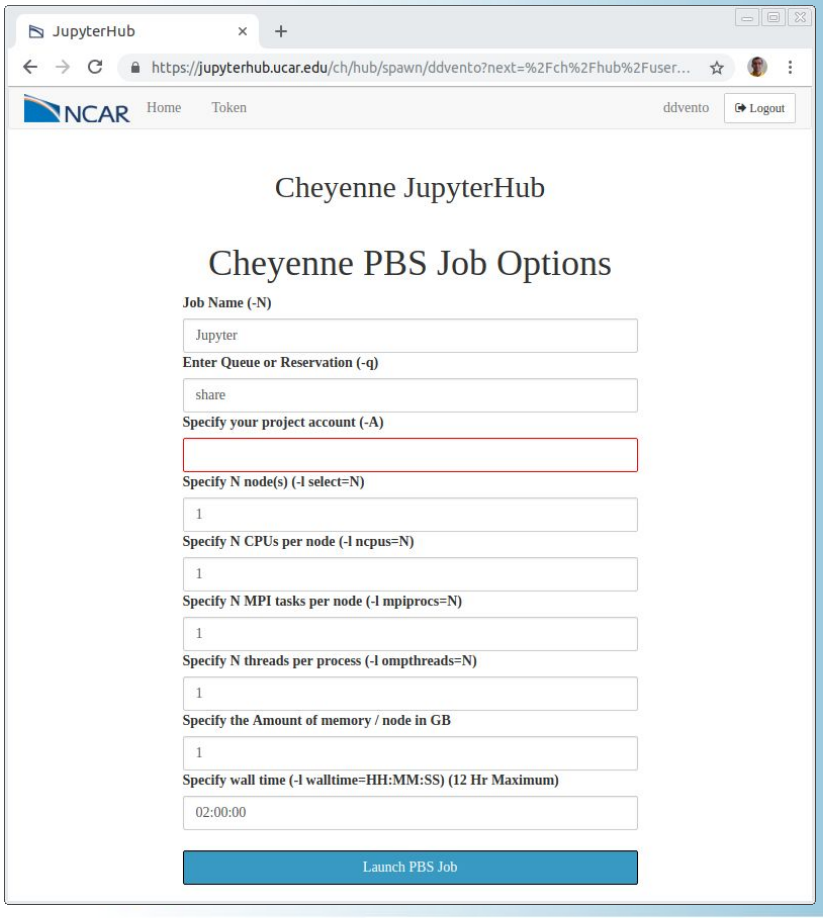
Submitting a PBS (or Slurm) job



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Why submitting a job?

- Your node, your resources…
- i.e. others will not step on your toes (& vice versa)

- The memory is yours, if you run out, you have exhausted hw
- CPU is yours, if you run out…
- GPU (if you requested) is yours...

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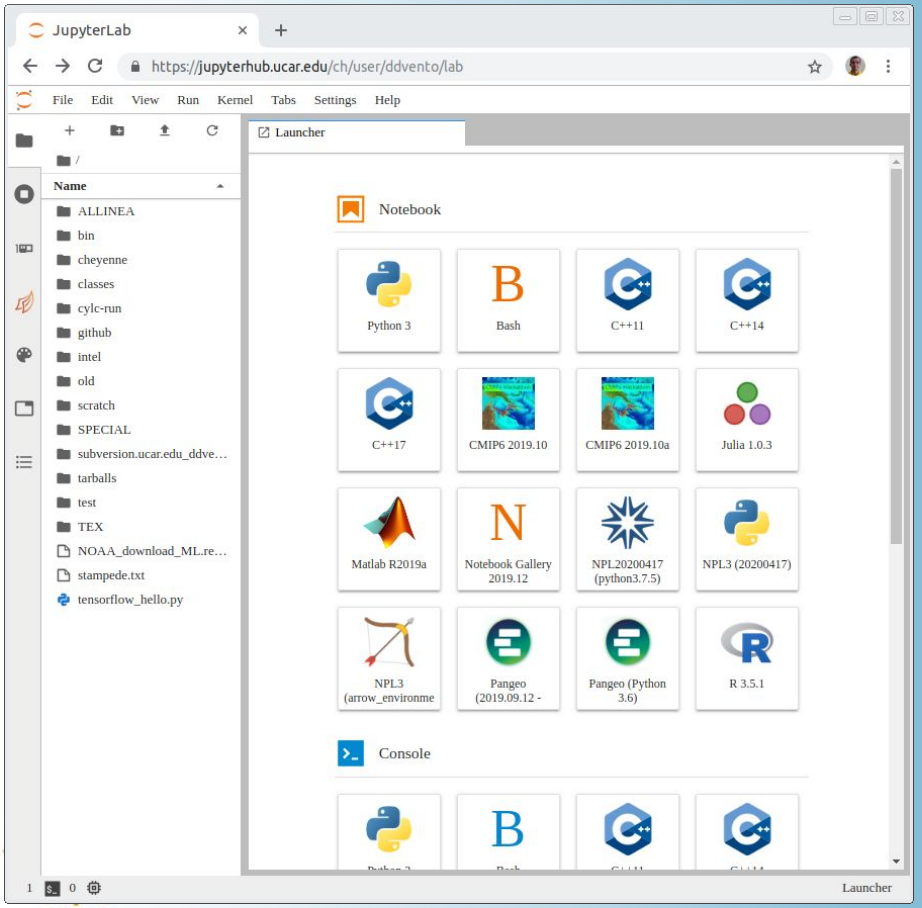
Launch a kernel



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What is a kernel?

- The kernel is a program which interprets what you type, execute it in the language of choice, and keep the “session” in scope (so variables are not forgotten at each RETURN)

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What kernels can you use?

- Three varieties (that I know of):
  - Provided by NCAR/CISL
    (actually two kinds of these, next slide)
  - Provided by you as mods of CISL's ones
  - Provided by you as conda environments

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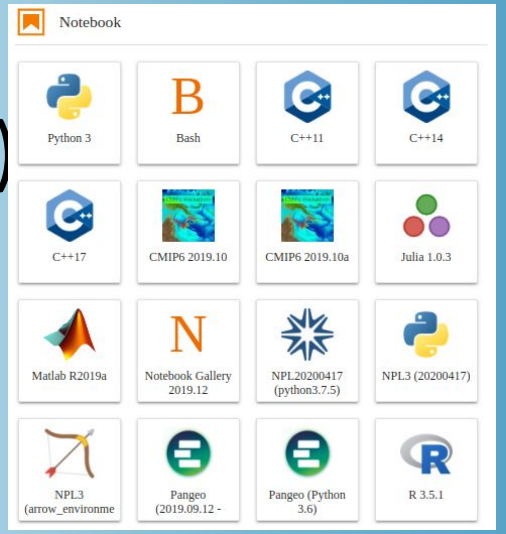
How to choose a kernel?

- What programming language would you like to use?
- Often Python, but many more are available (C, julia, matlab..)
- What libraries do you need?



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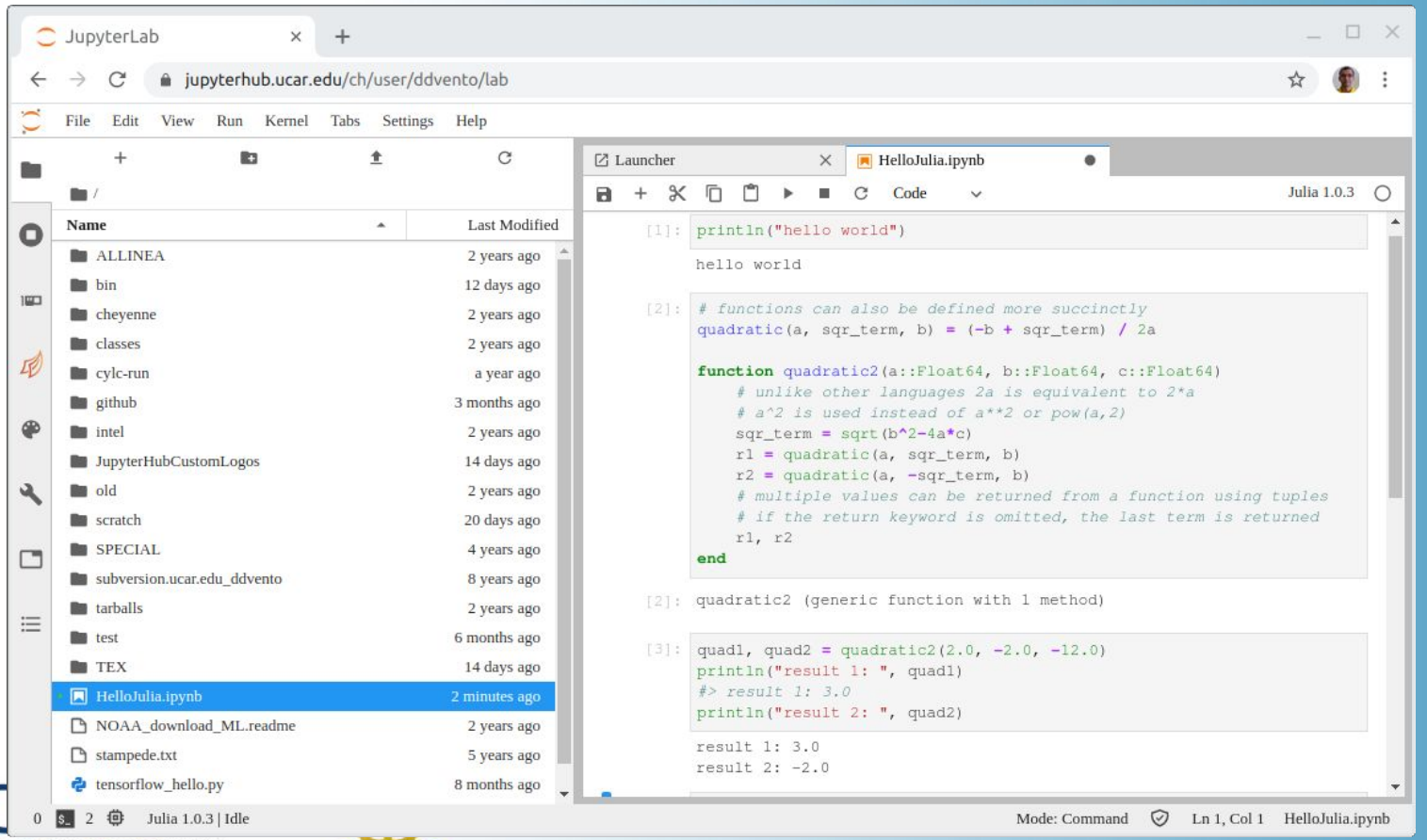
Working with a notebook



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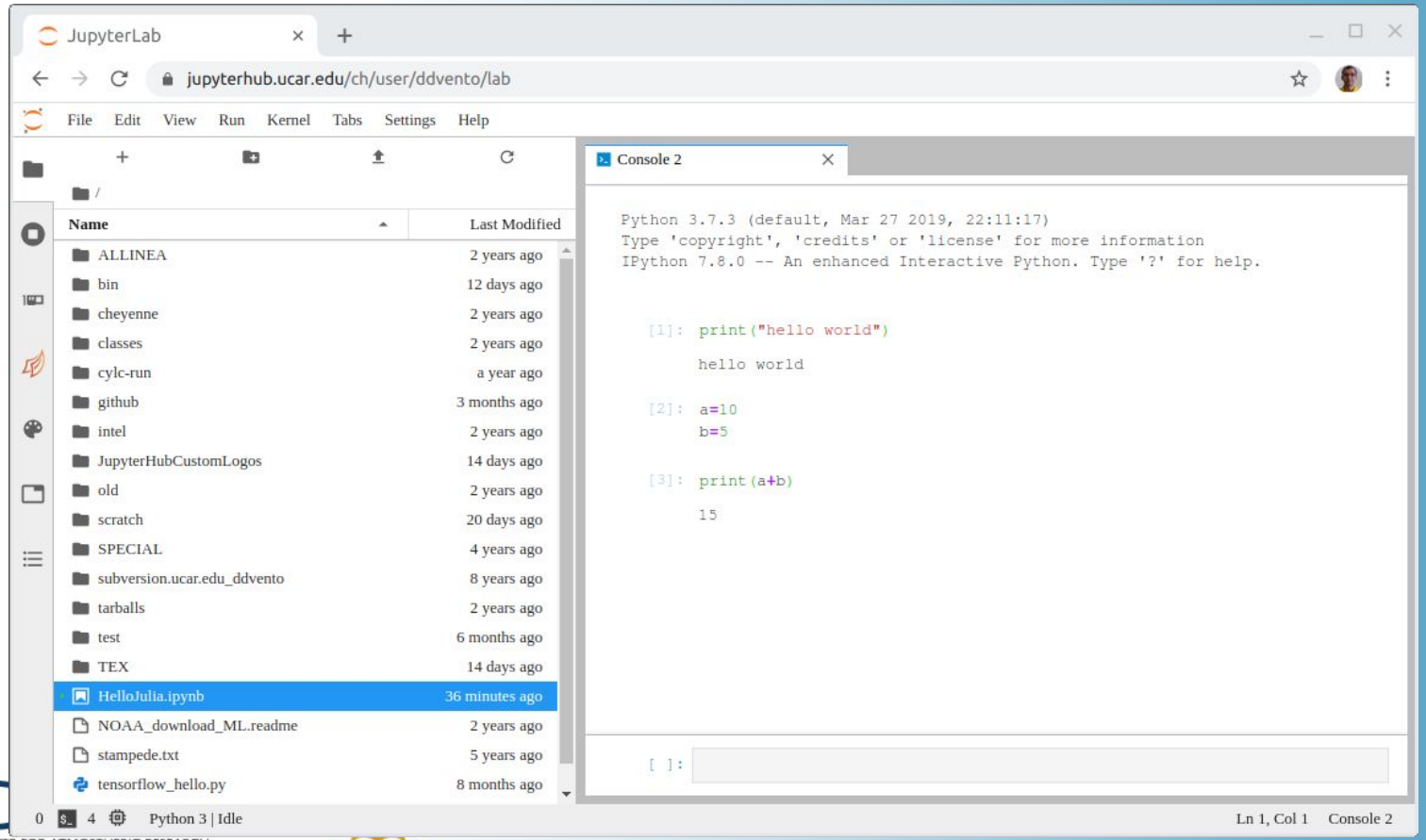
Working with the console



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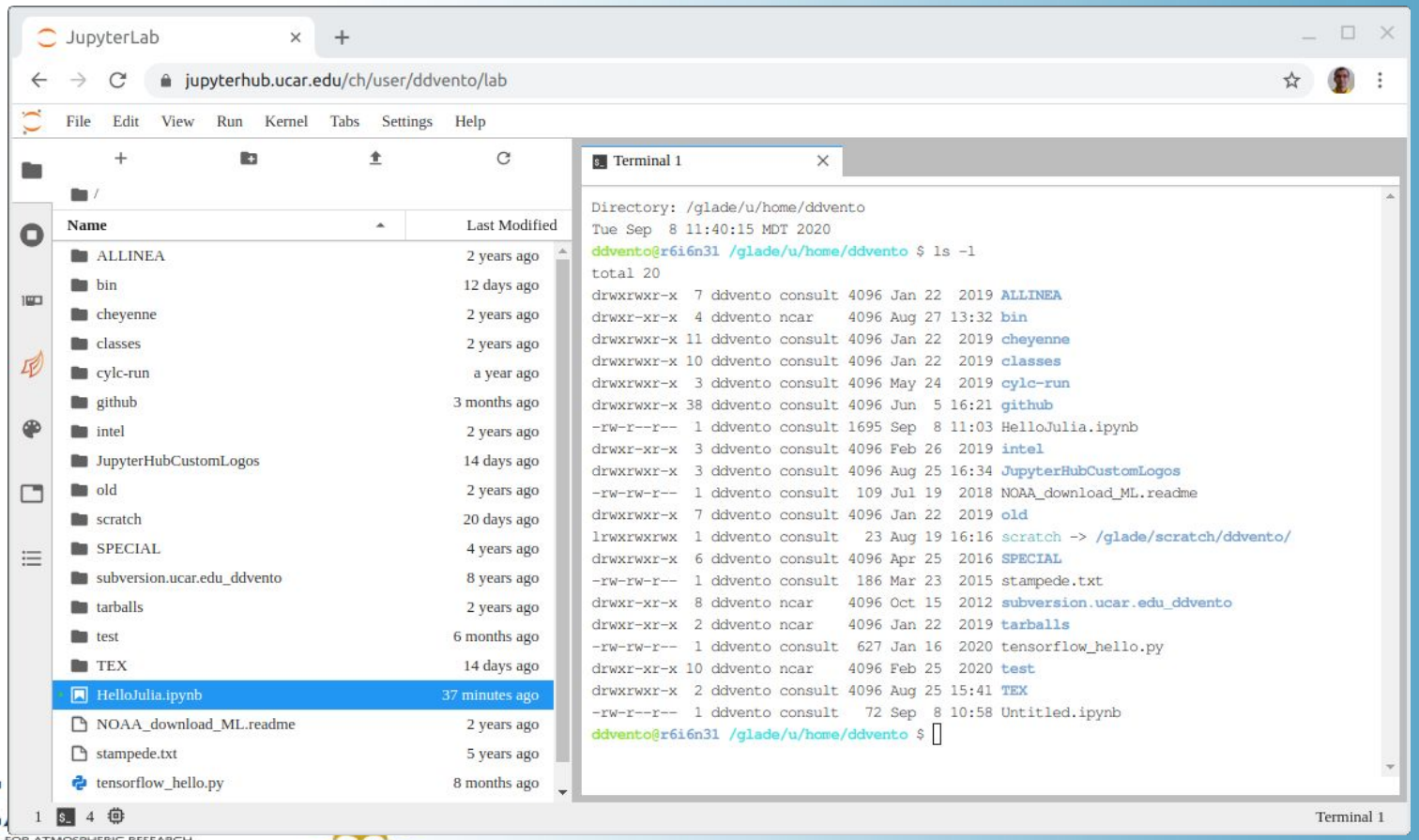
Working with the shell



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Back to presentation

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