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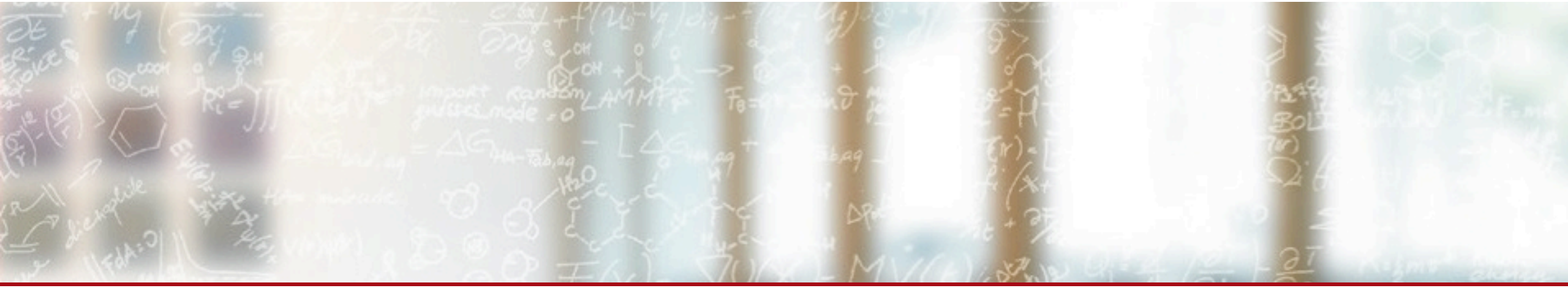


Interactive Computing with JupyterLab, IJulia and IPyParaview

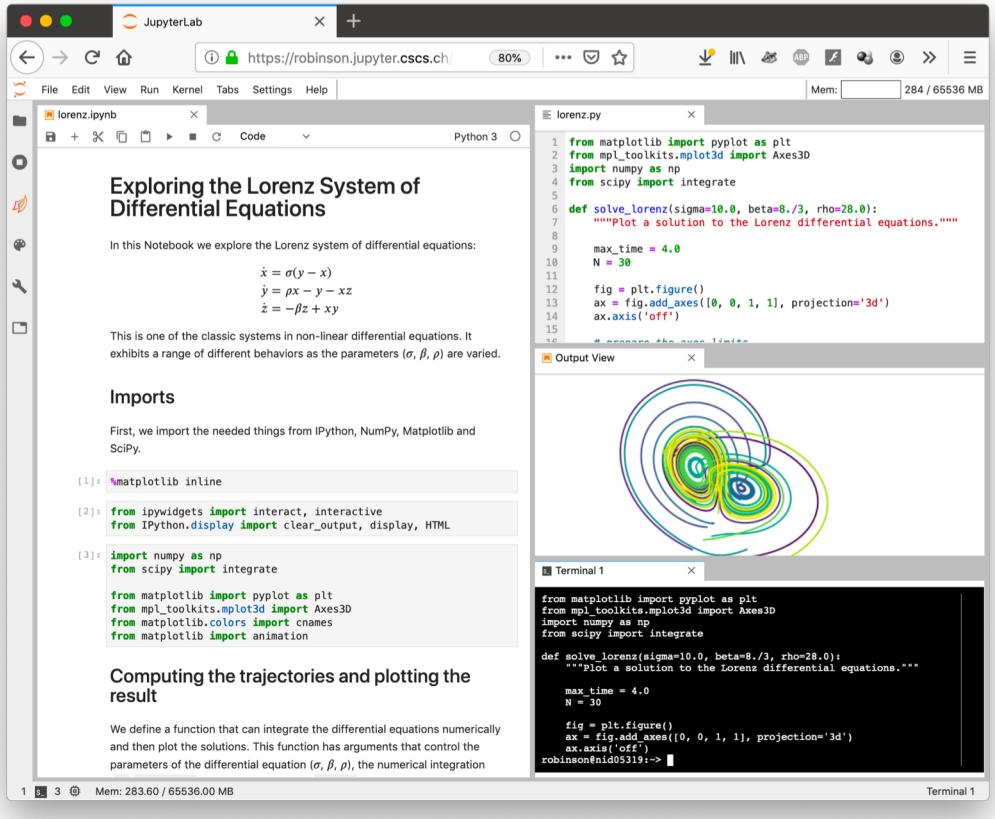
Tim Robinson
Sam Omlin
Jean Favre

Agenda

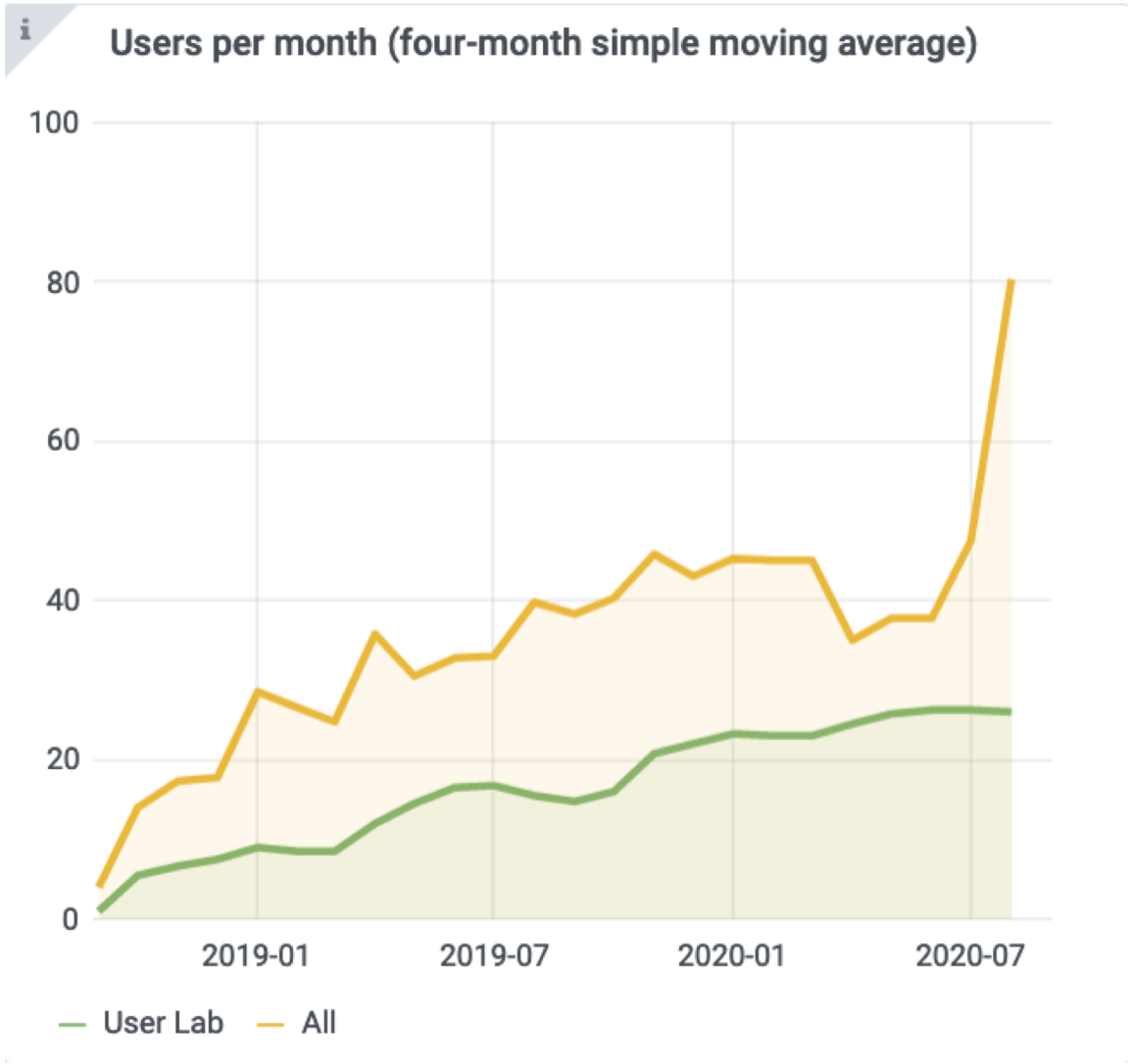
- New functionality in JupyterLab
  - GPU dashboards
  - Code formatting with Black
  - Creating a custom kernel
- IJulia kernel for using Julia in JupyterLab
- ParaView for visualization in JupyterLab

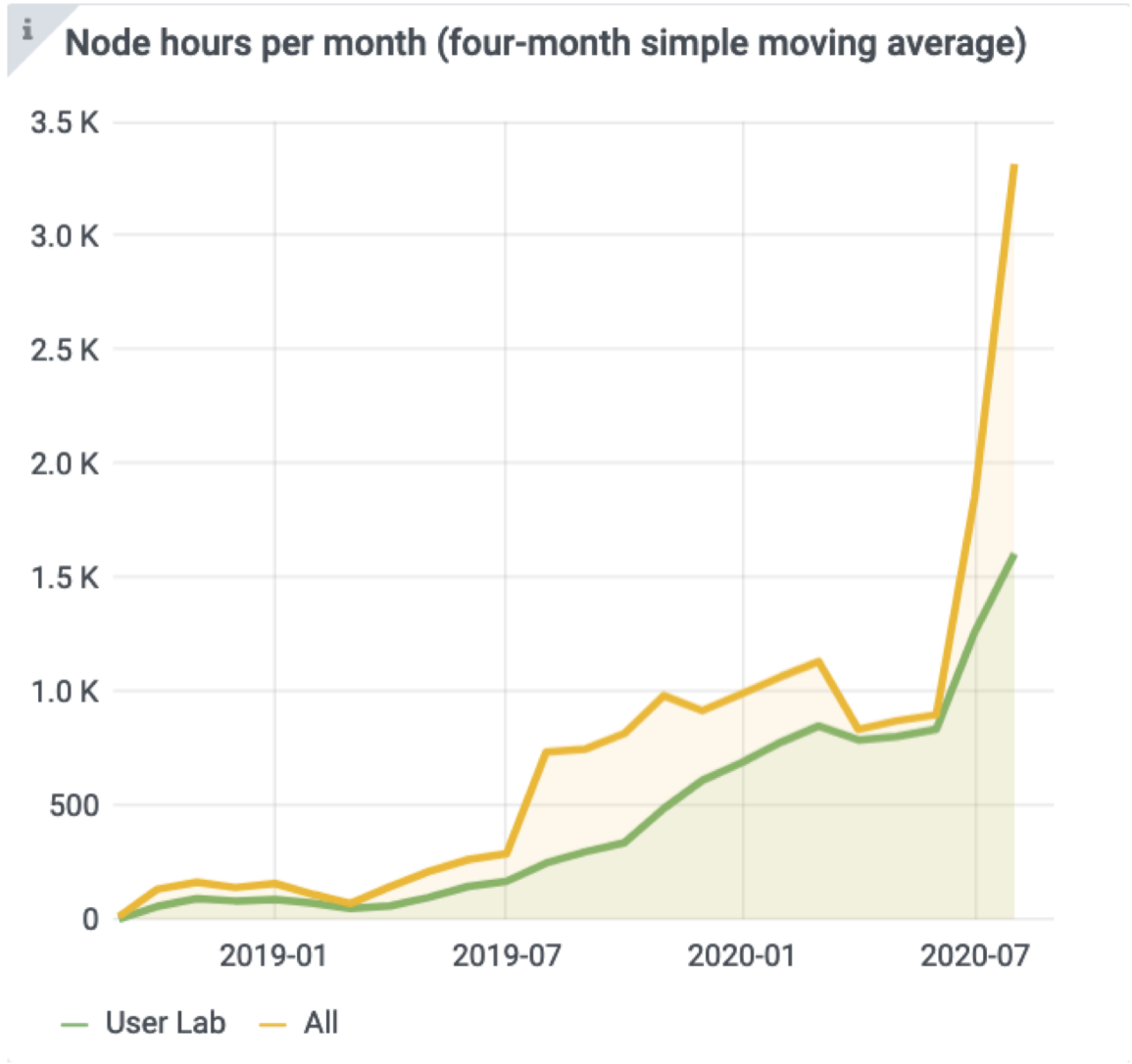
JupyterLab on Piz Daint

- JupyterHub provides JupyterLab servers on demand at https://jupyter.cscs.ch
- Anyone with access to Piz Daint can log in with their CSCS credentials (Kerberos/LDAP)
- Servers are launched on compute nodes of Piz Daint (GPU or multicore)
- You have dedicated access to the full compute capability of the node
- Special queues for interactive computing grow and shrink automatically according to demand



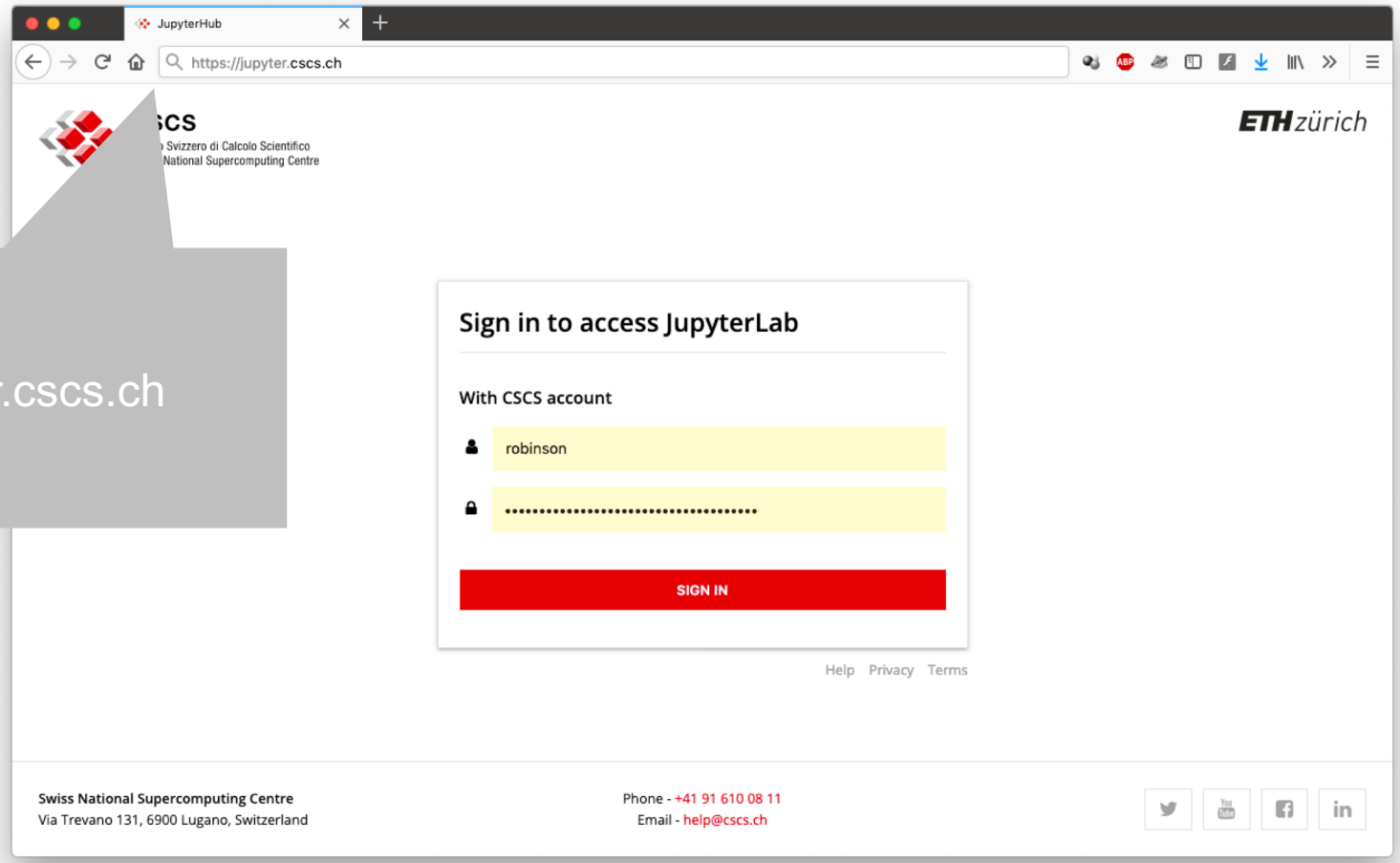
JupyterLab usage over time



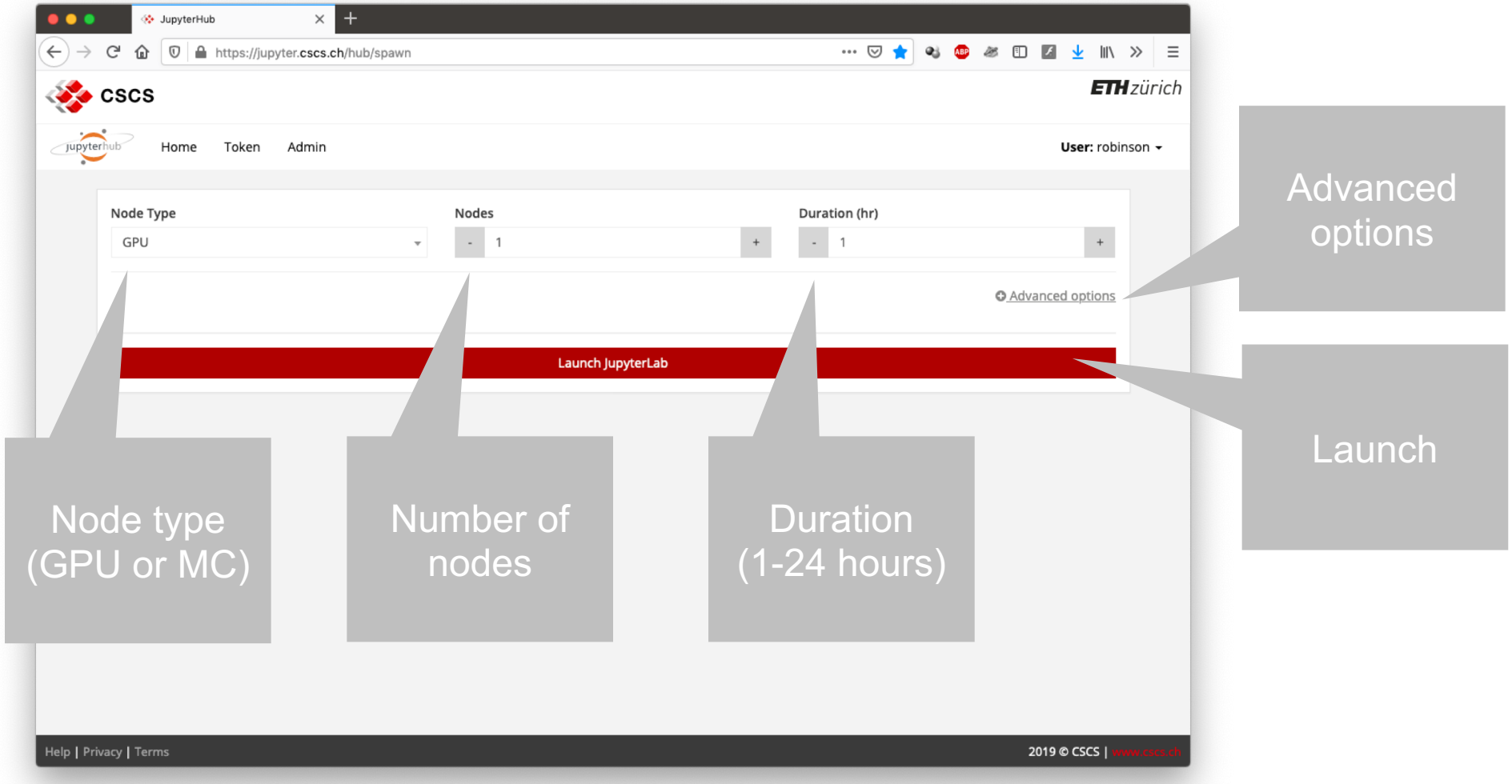


Logging in

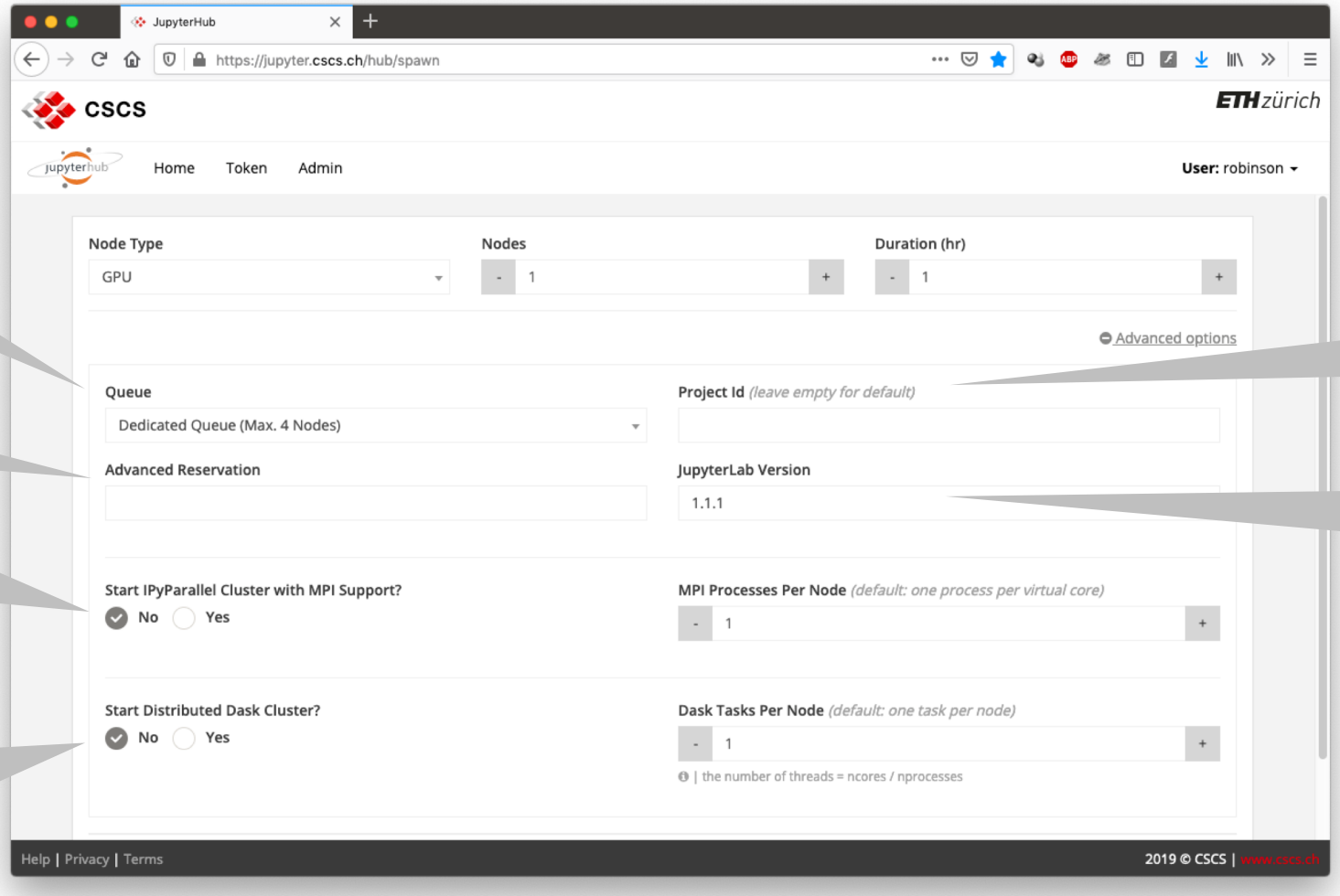
https://jupyter.cscs.ch



Basic options



Advanced options



Queue

Reservation

IPyParallel (multi-node notebooks)

Distributed Dask cluster (multi-node notebooks)

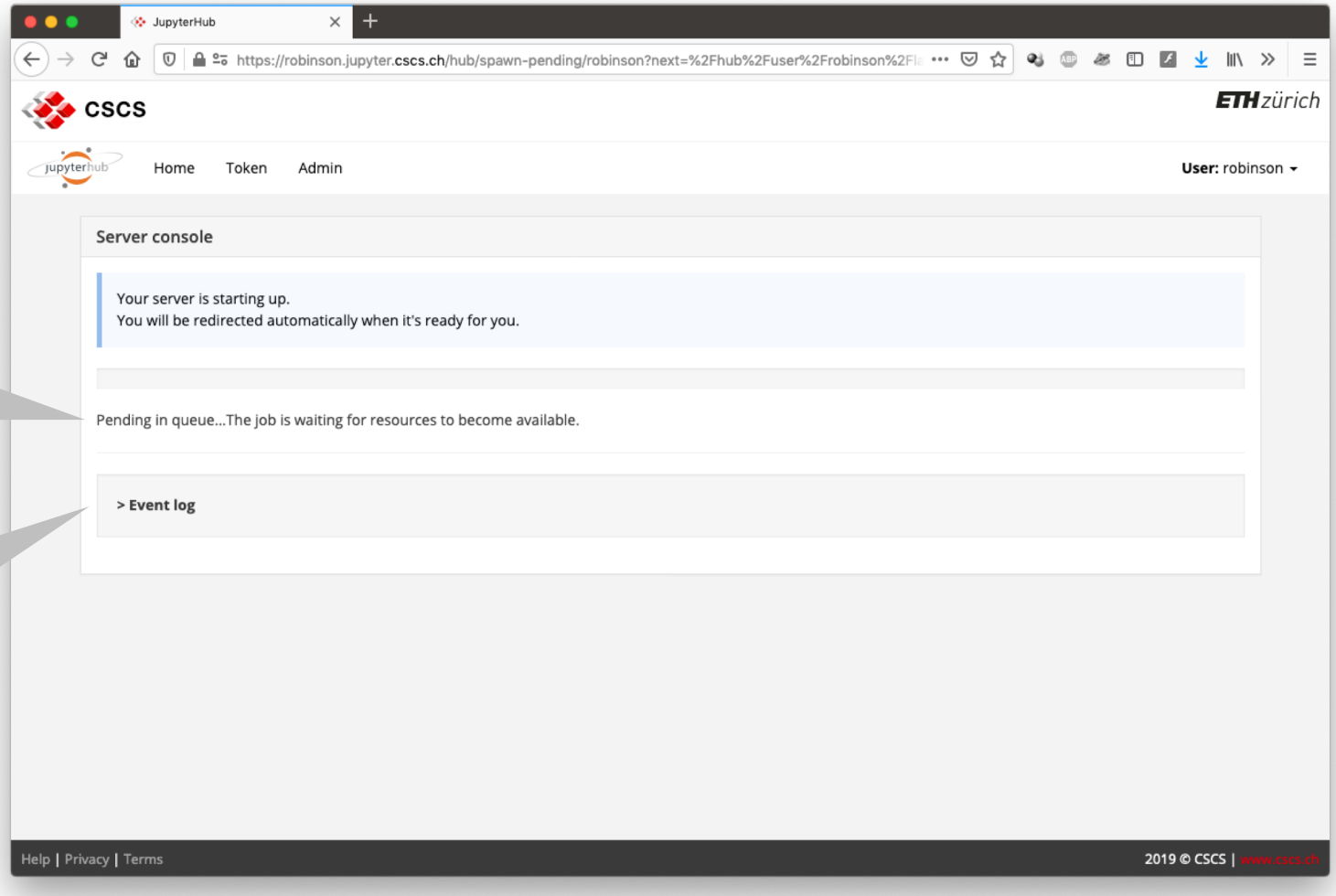
Project Id (account)

JupyterLab version

Launching

Progress

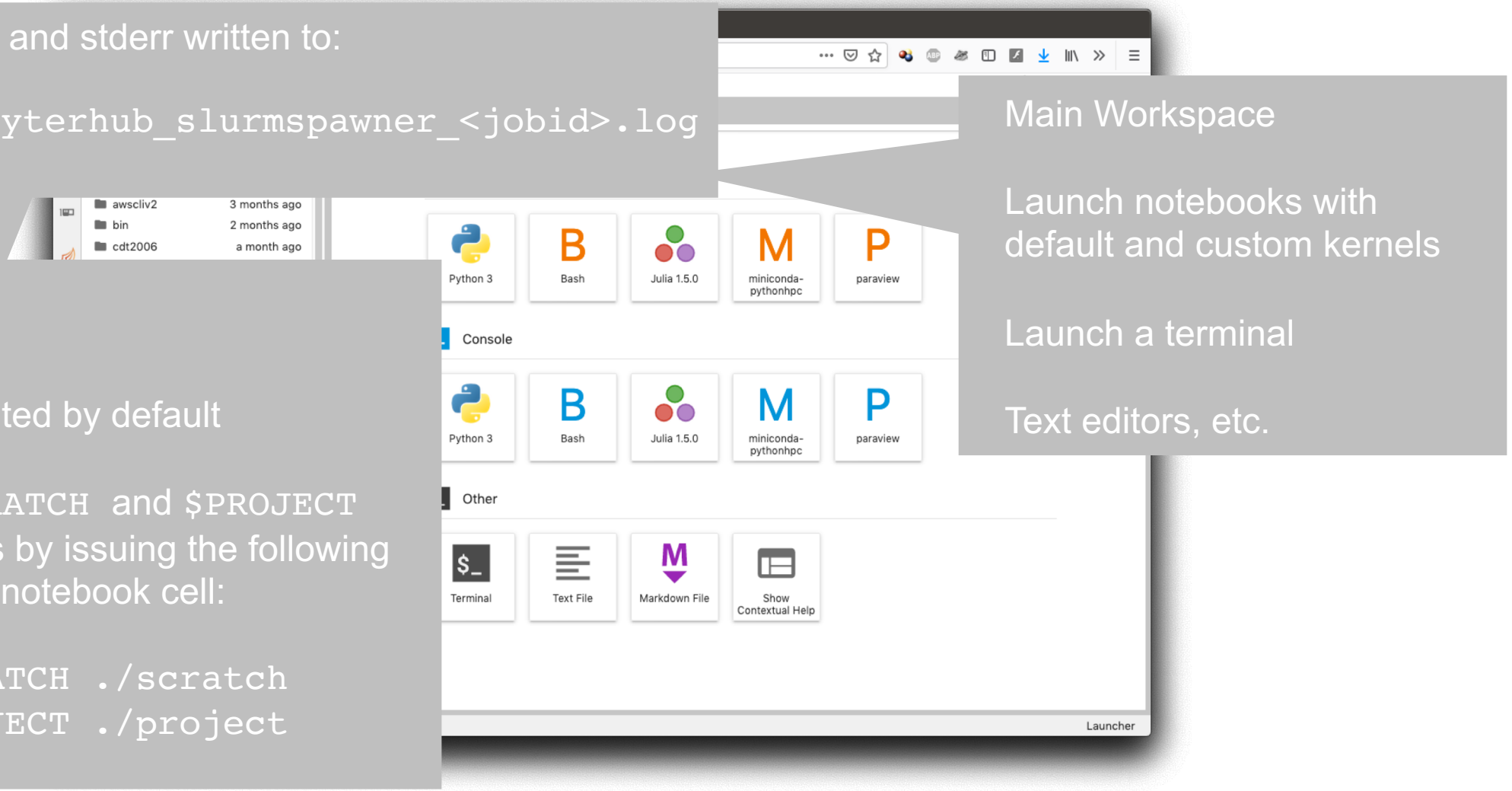
Event log



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
```

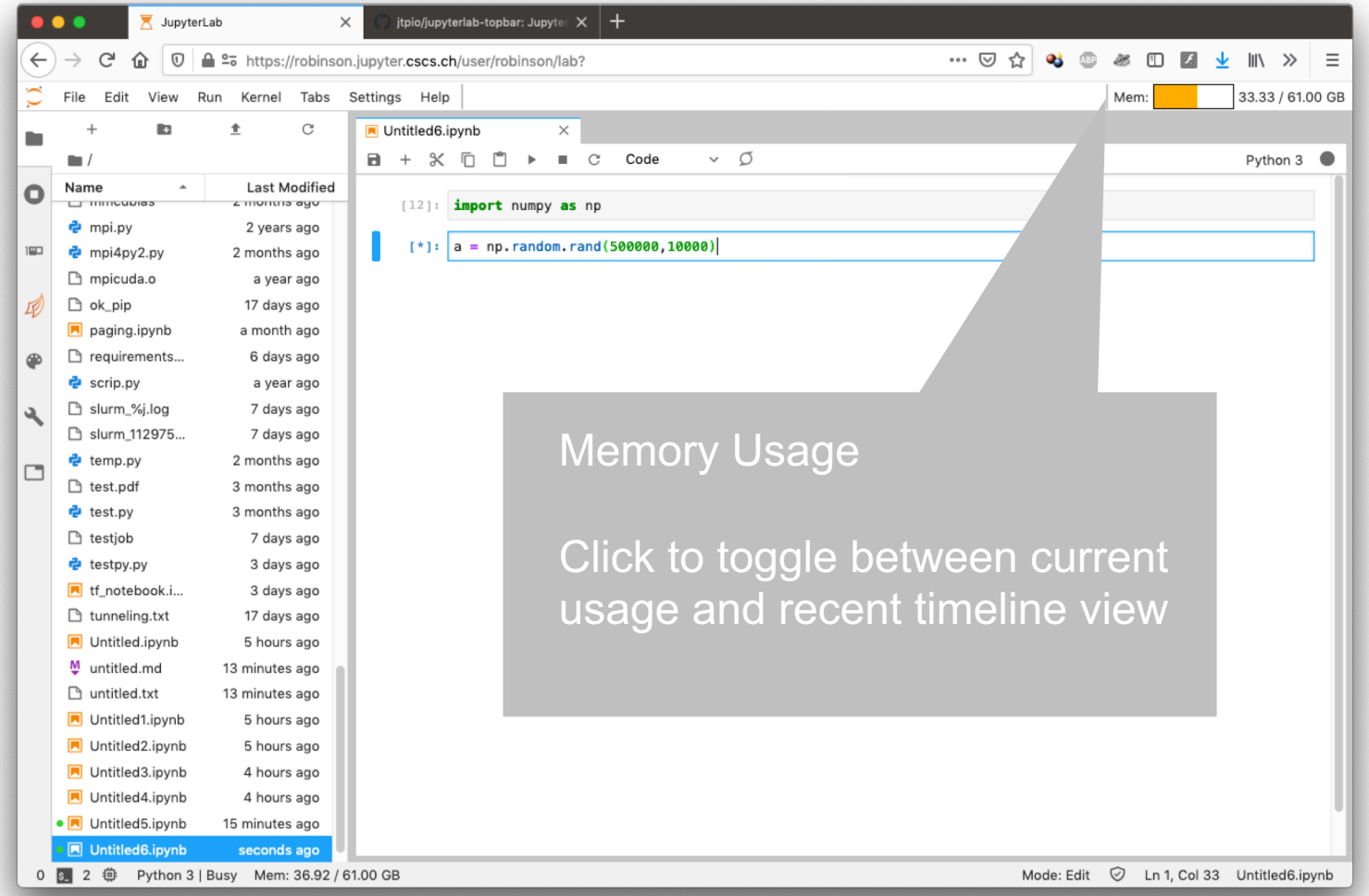
Main Workspace

Launch notebooks with default and custom kernels

Launch a terminal

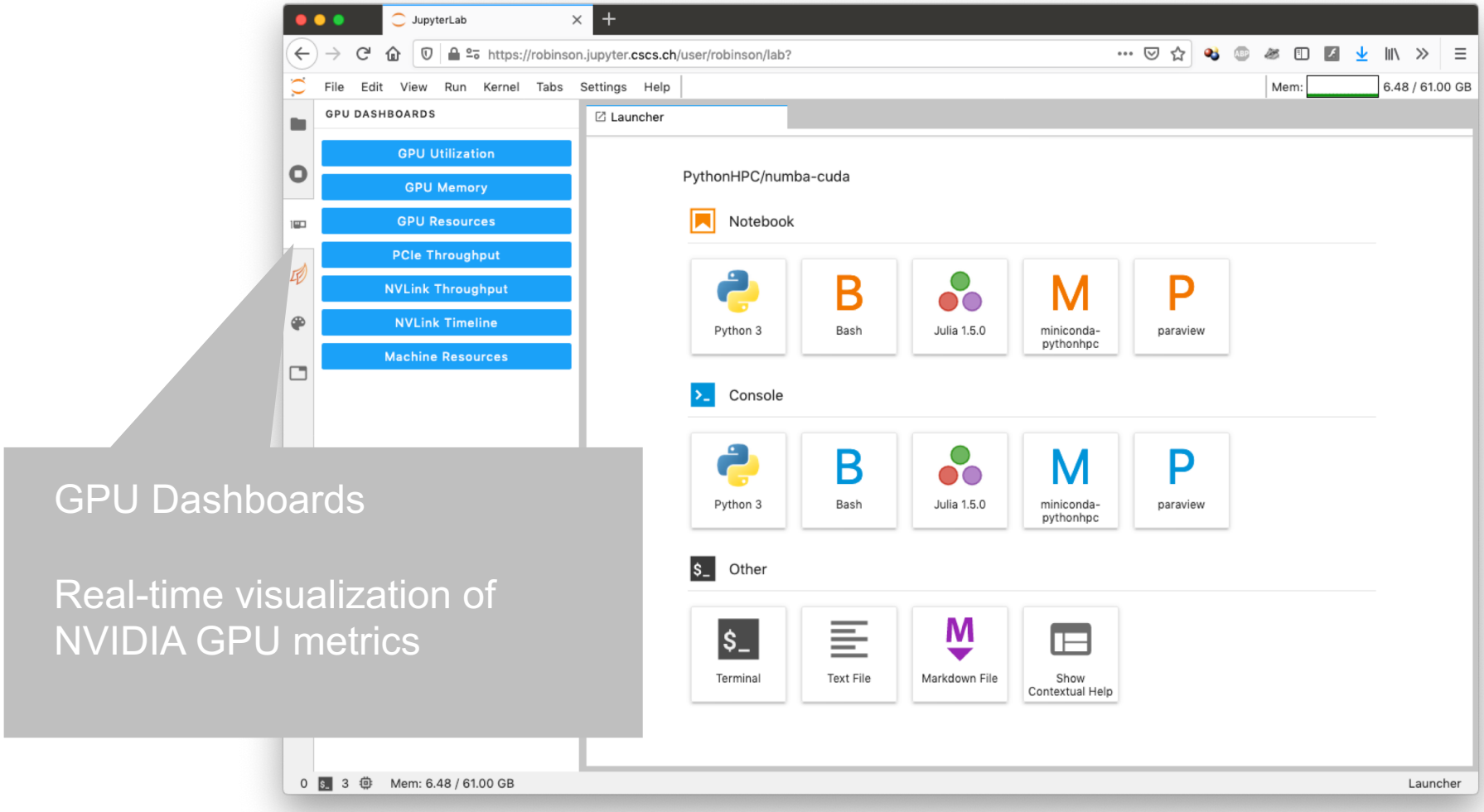
Text editors, etc.

Memory usage monitor

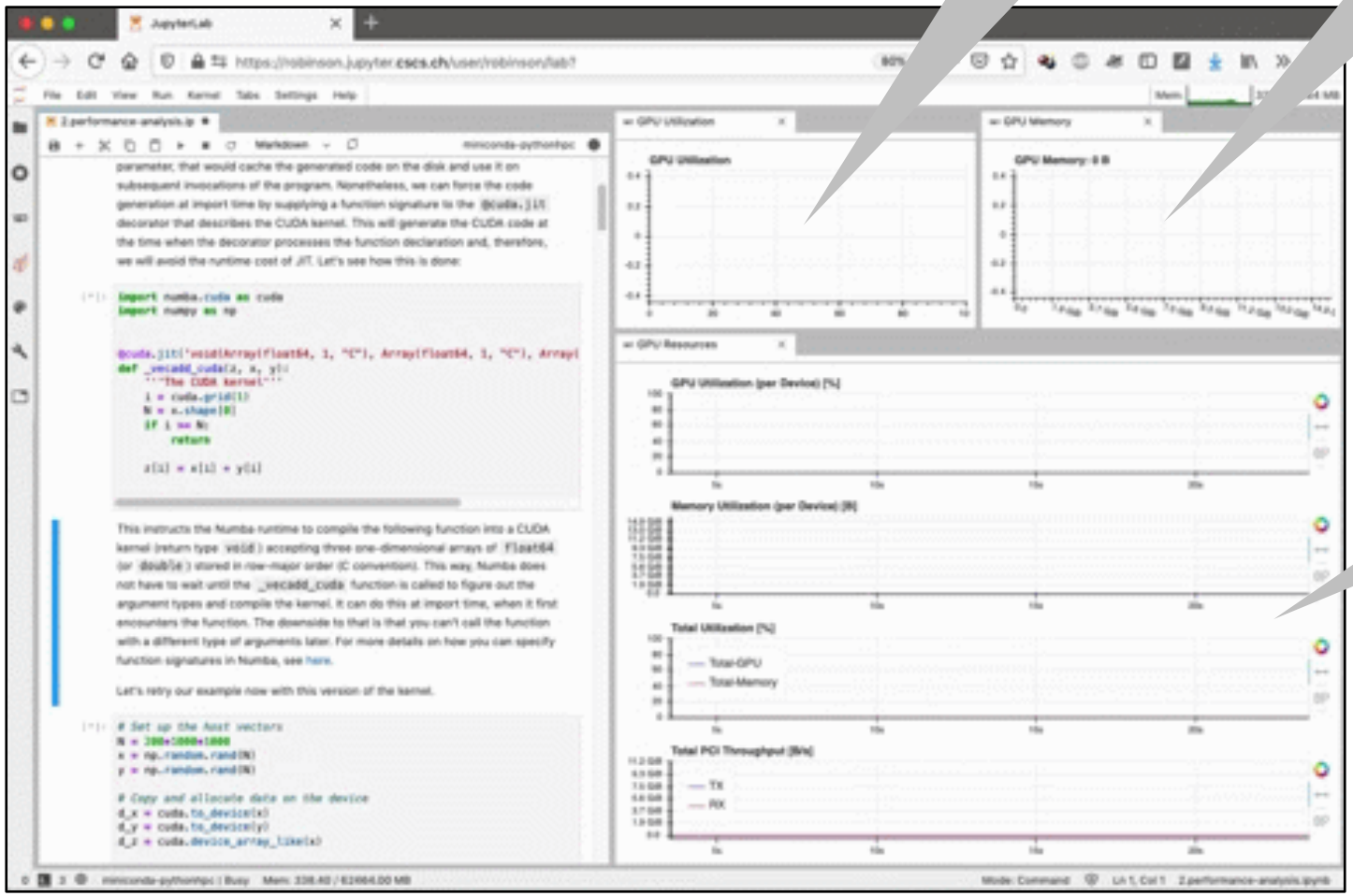


GPU dashboards

GPU dashboards

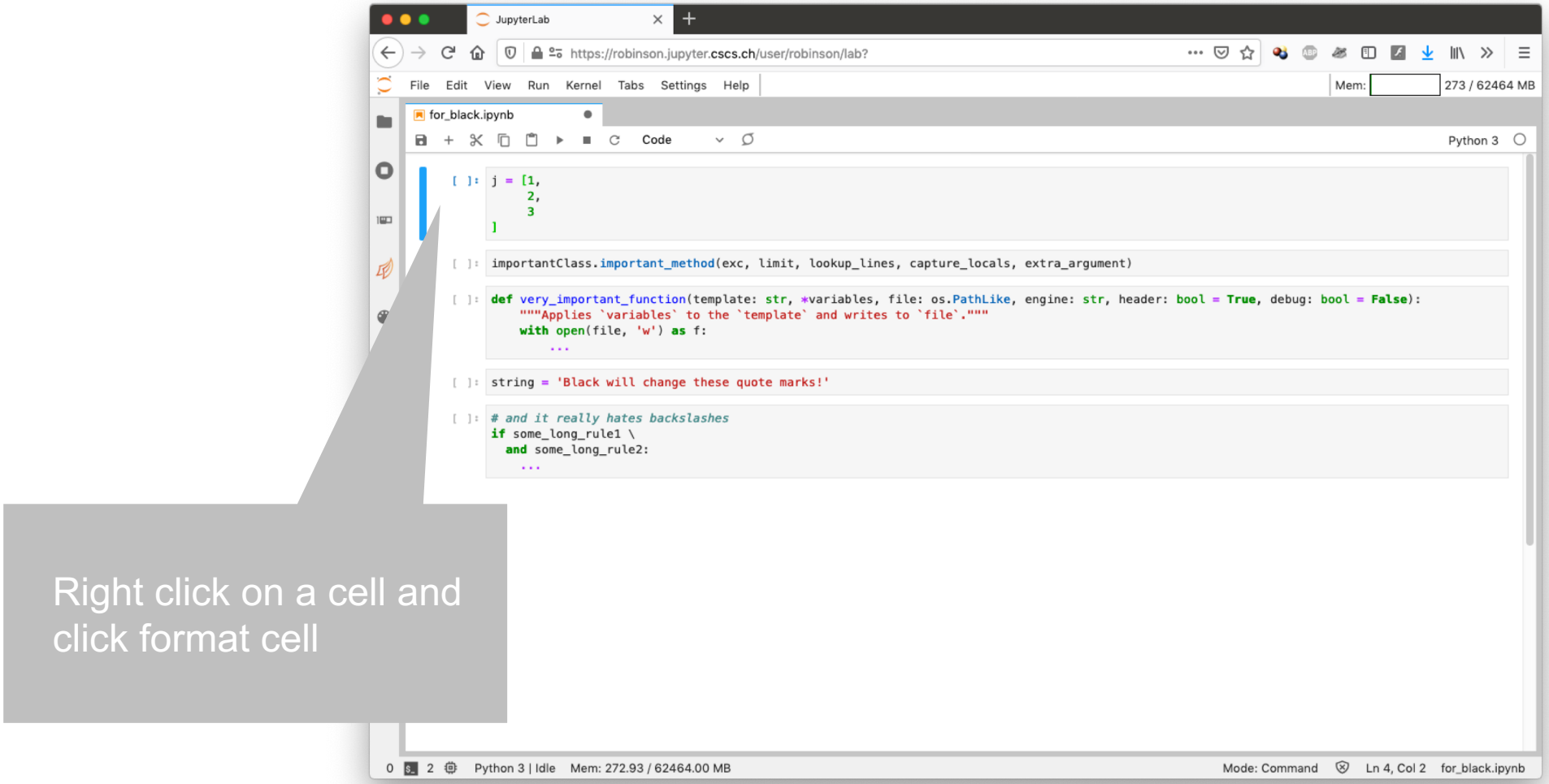


GPU dashboards



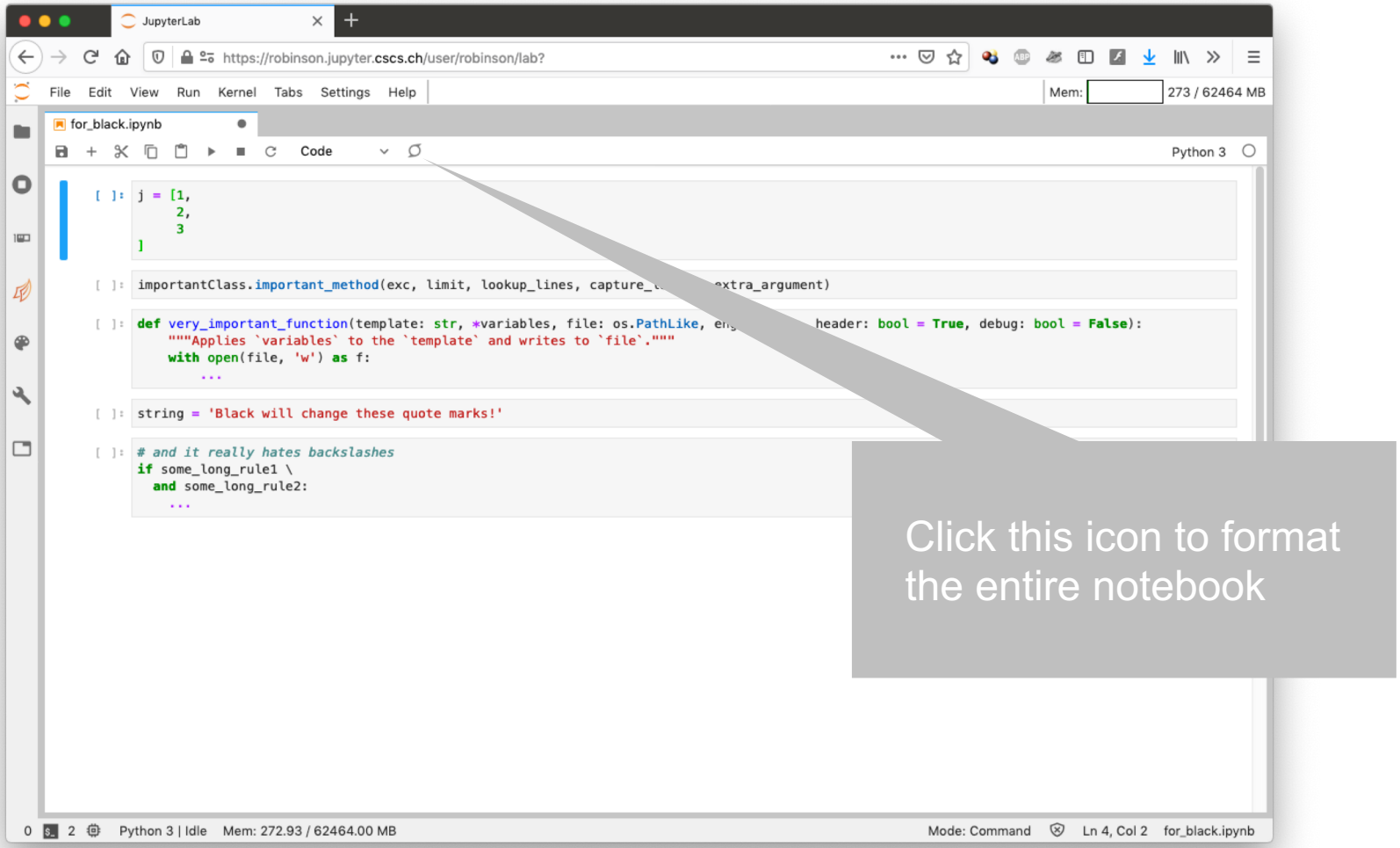
JupyterLab code formatter

Code formatter

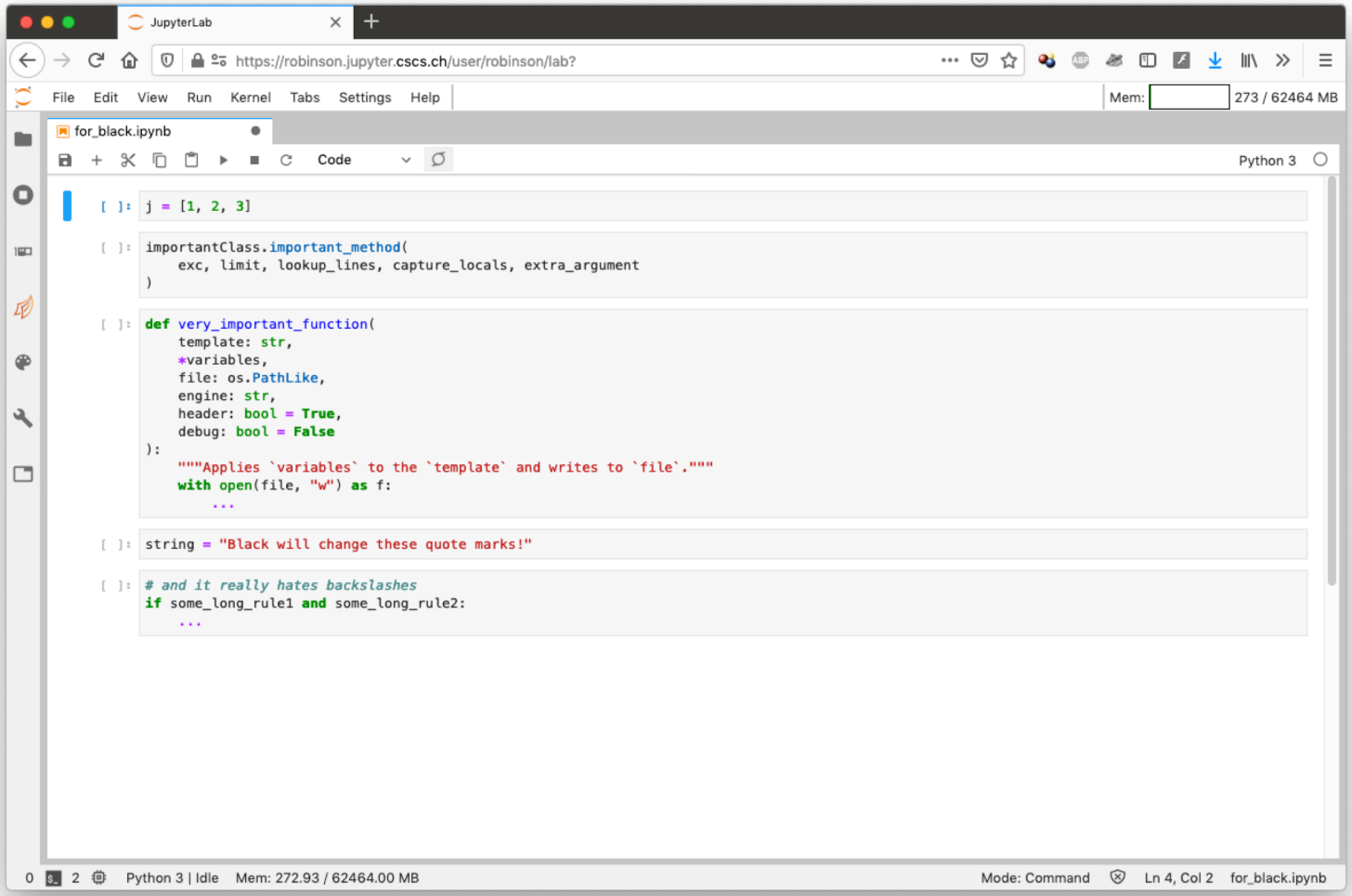


Right click on a cell and click format cell

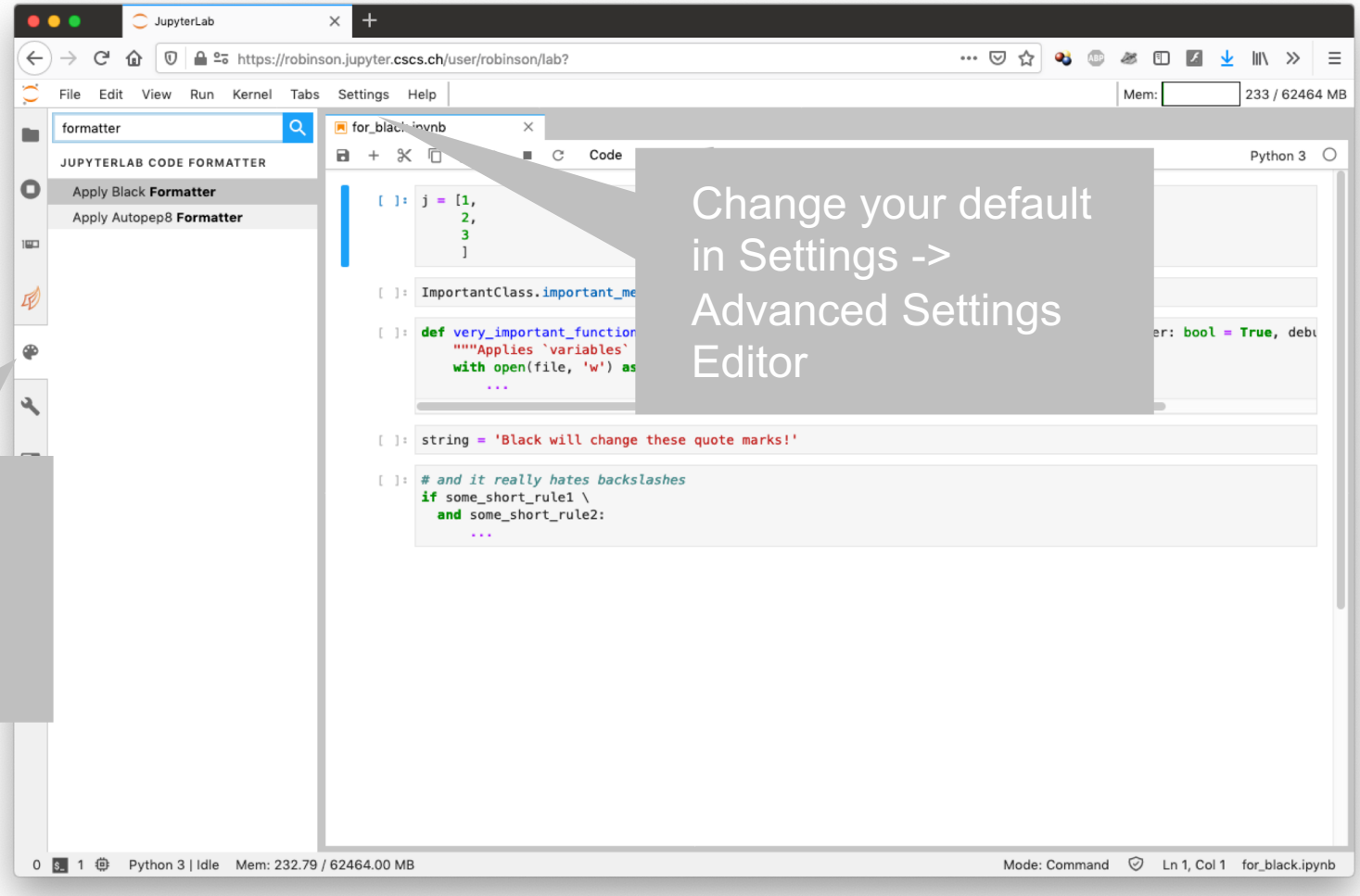
Code formatter



Code formatter



Code formatter

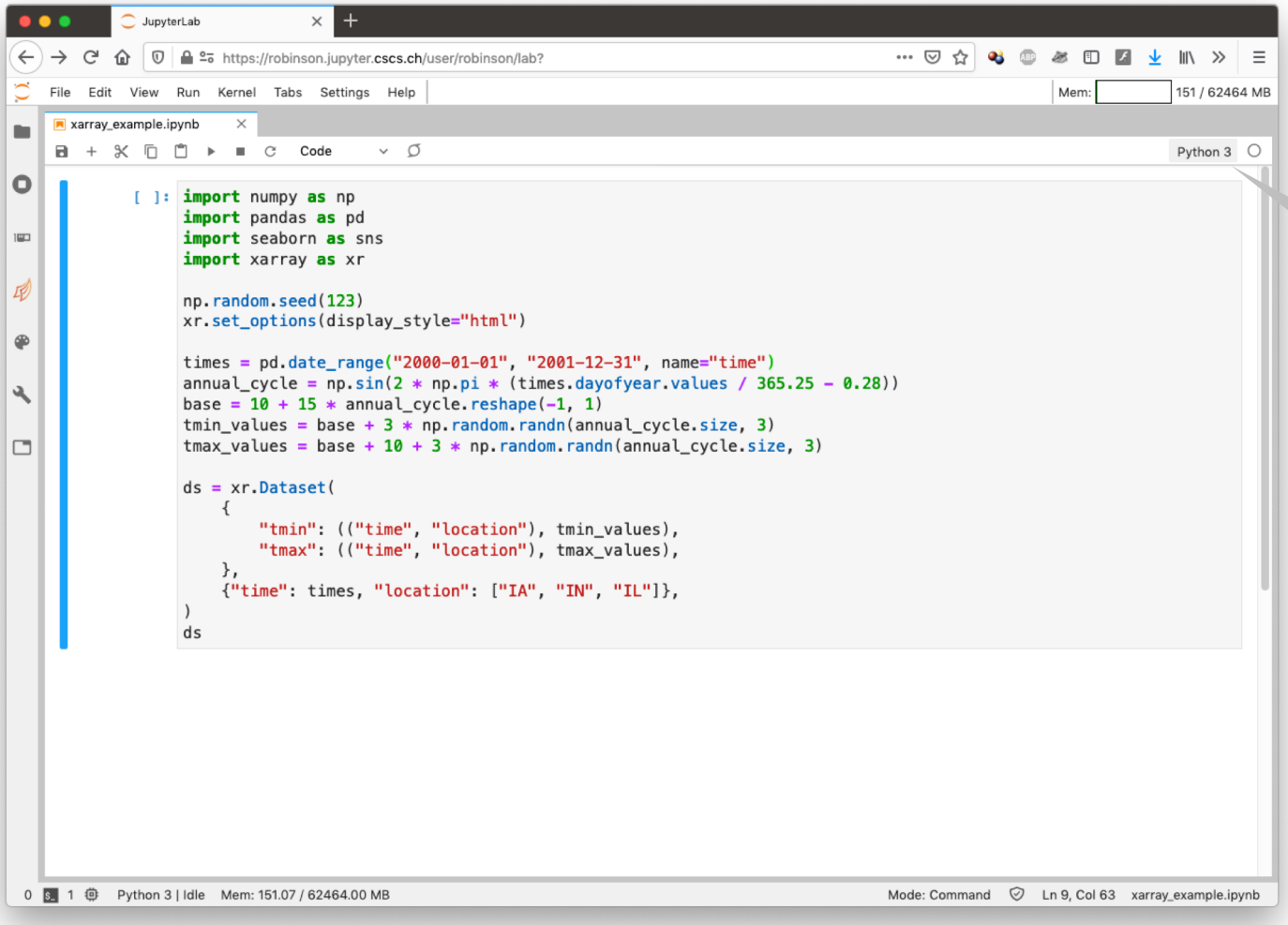


Select your own formatter in the command palette

Change your default in Settings -> Advanced Settings Editor

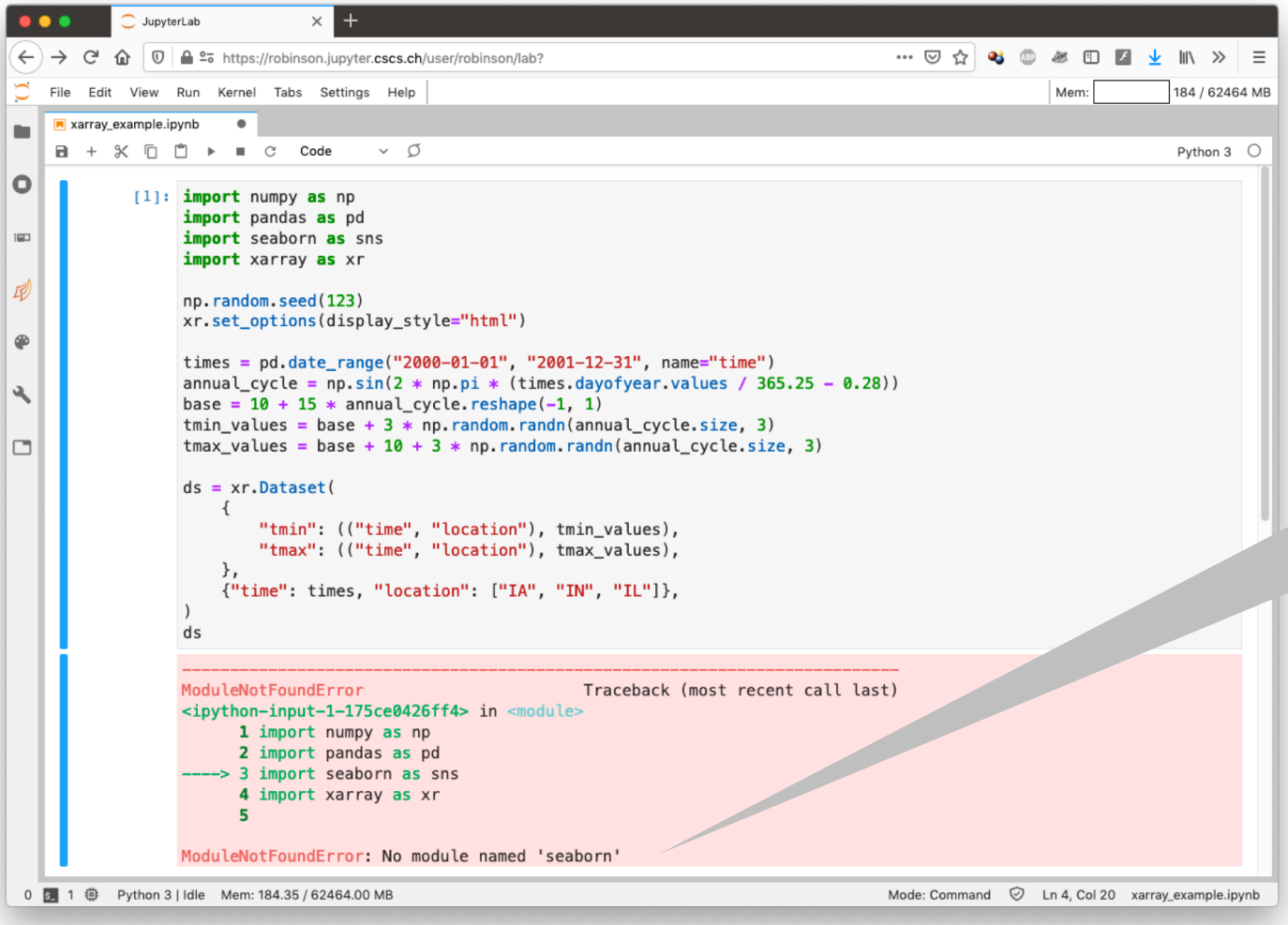
Customizing your Python environment

Adding Python modules with pip



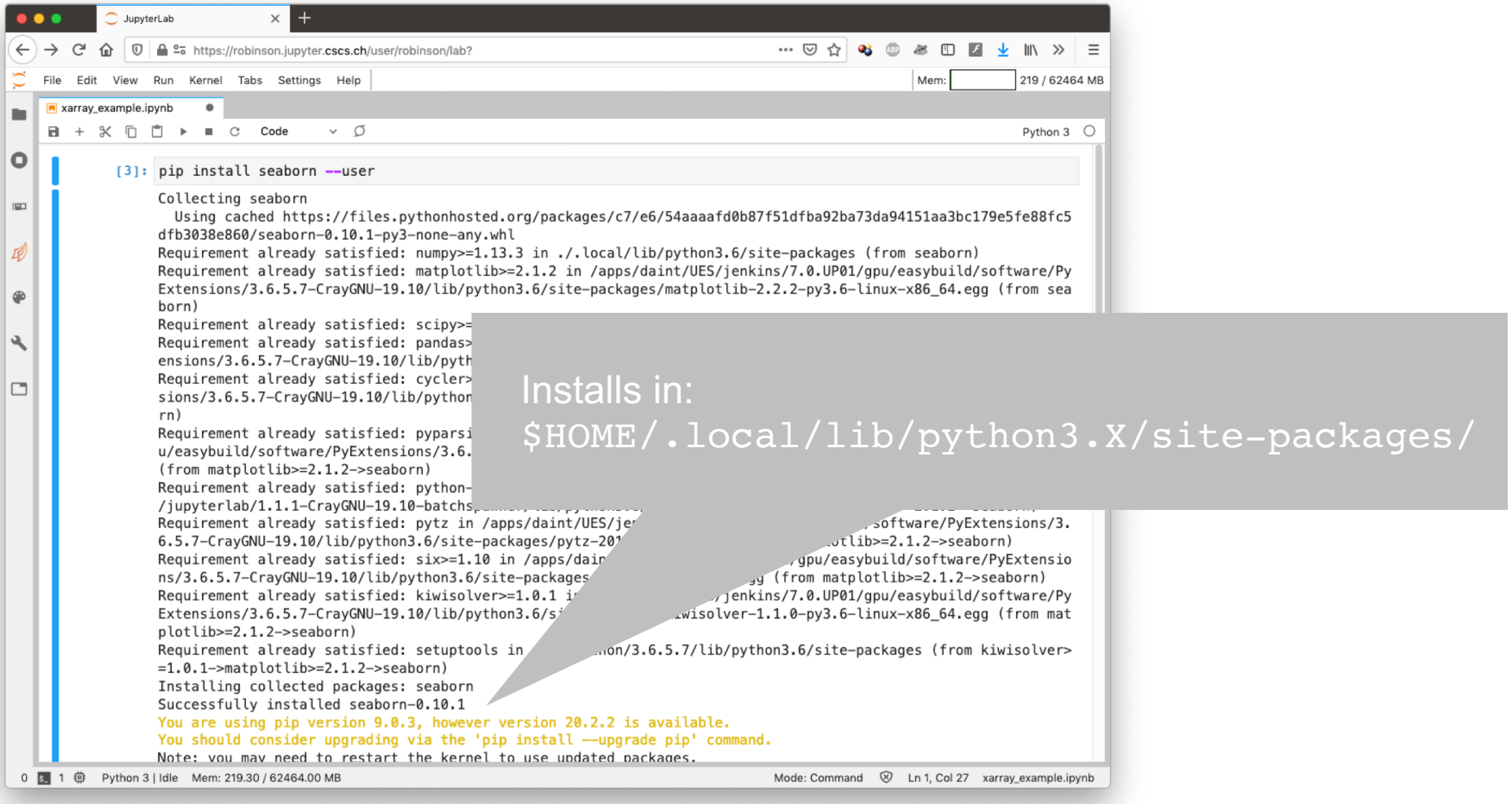
Default kernel: “Python 3”

Adding Python modules with pip

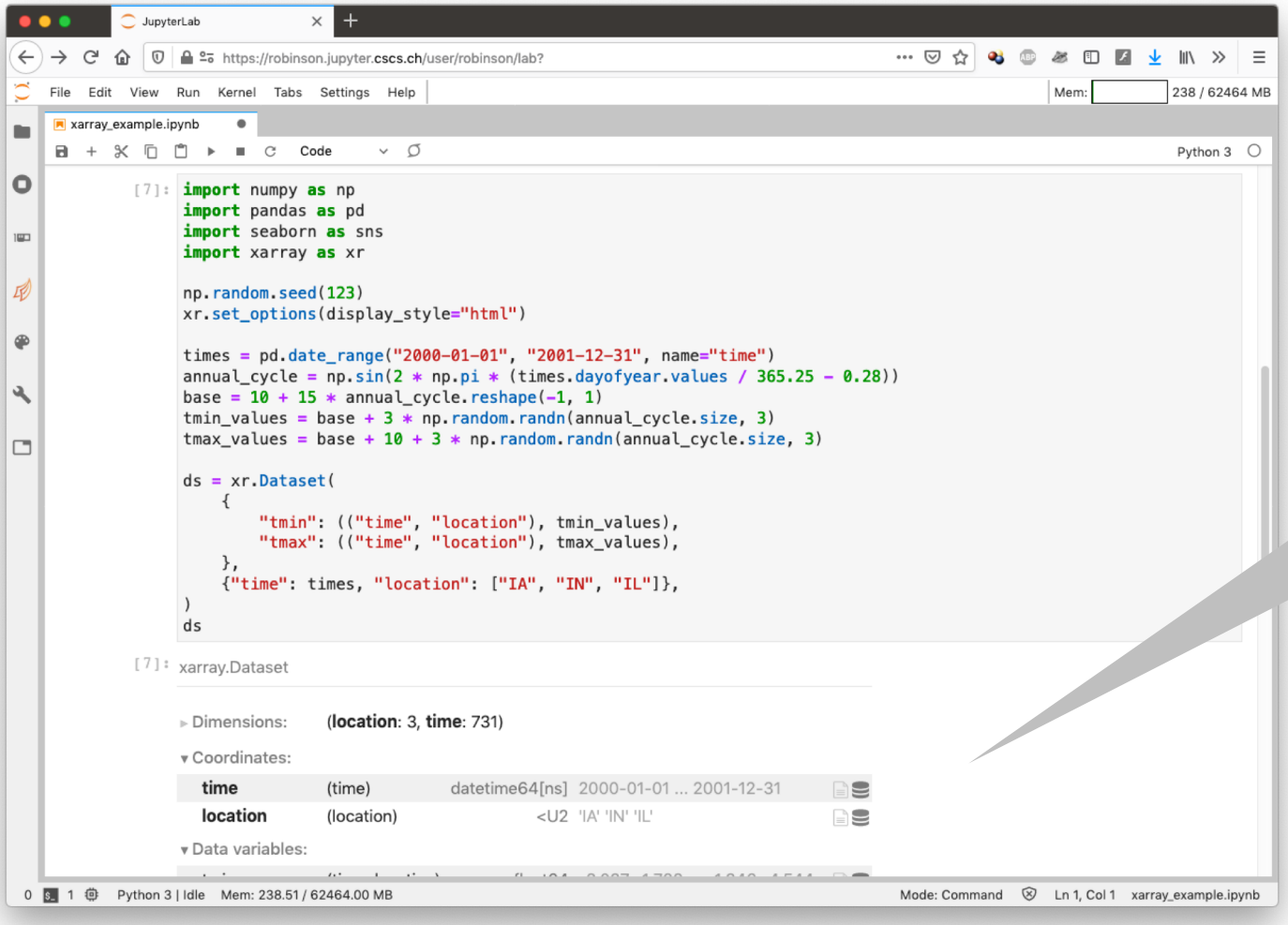


Missing: `seaborn`, `xarray`, ...

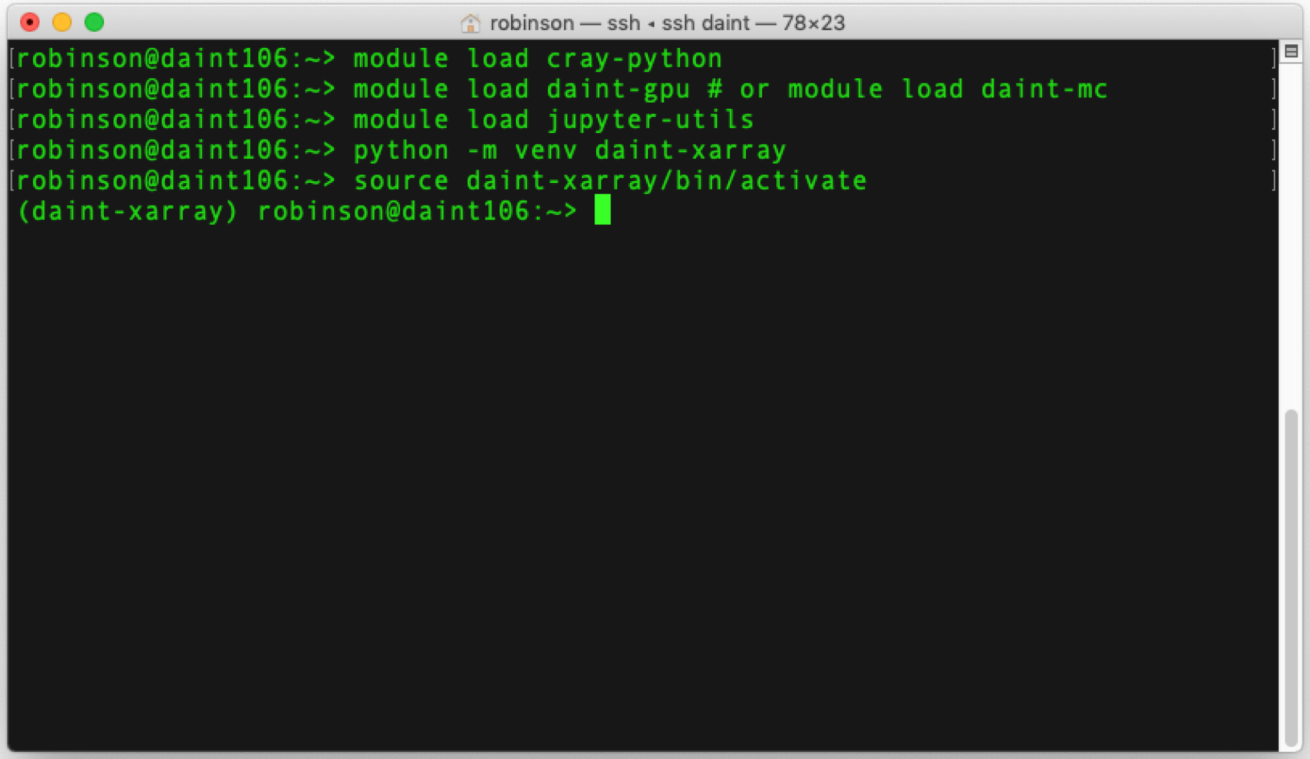
Adding Python modules with pip



Adding Python modules with pip



Creating and installing a custom kernel (recommended)



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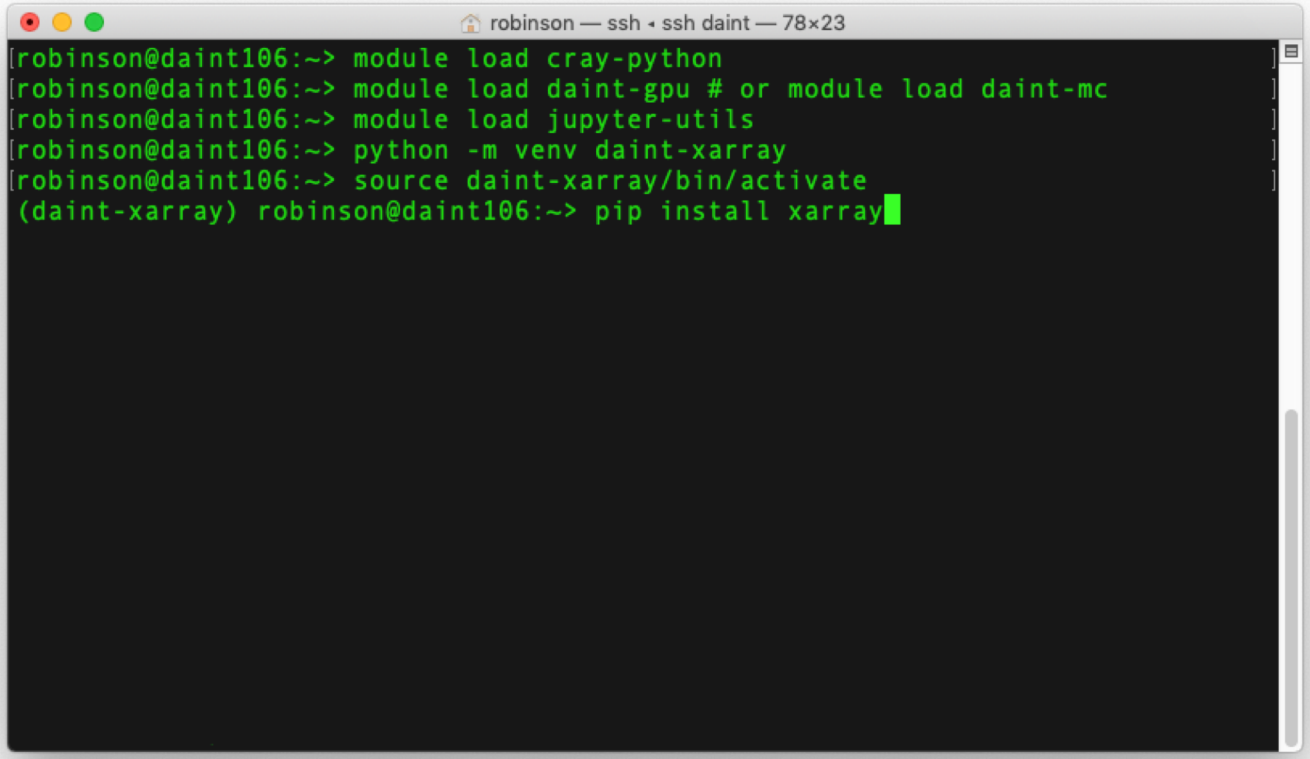

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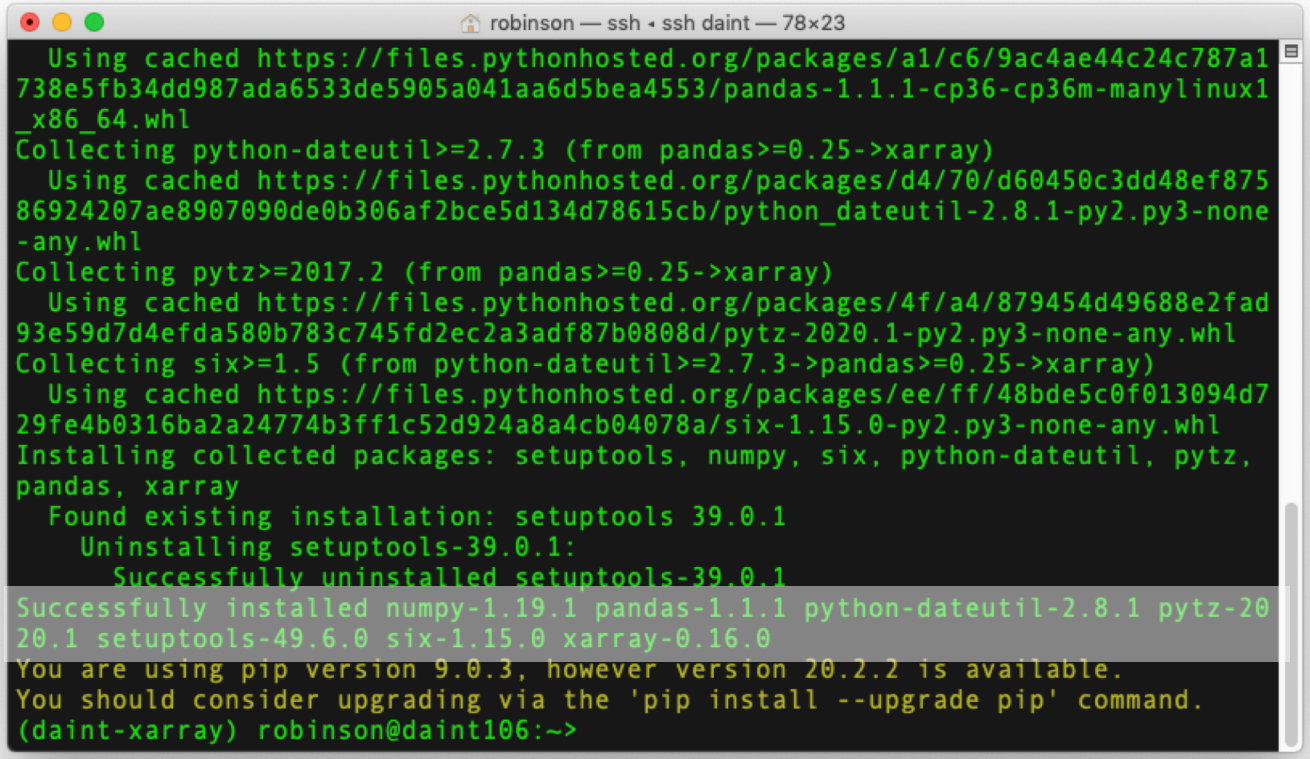

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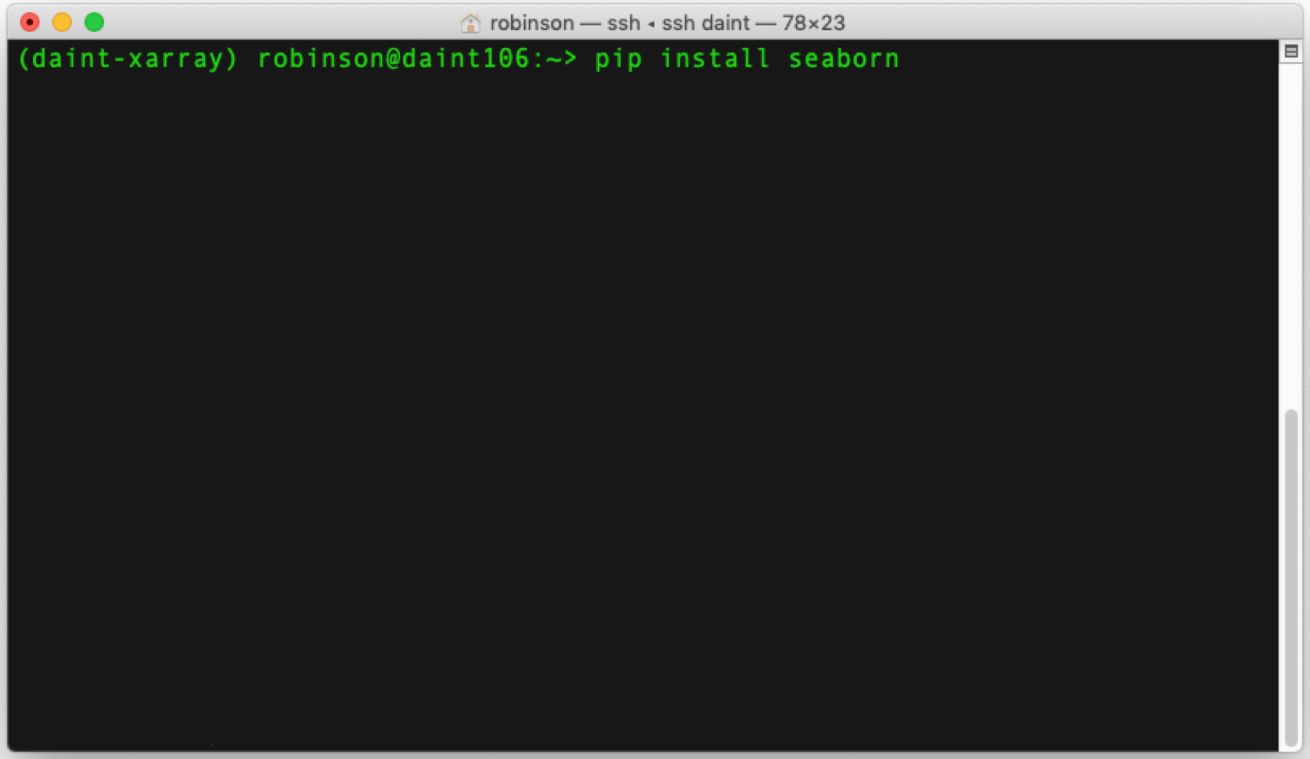

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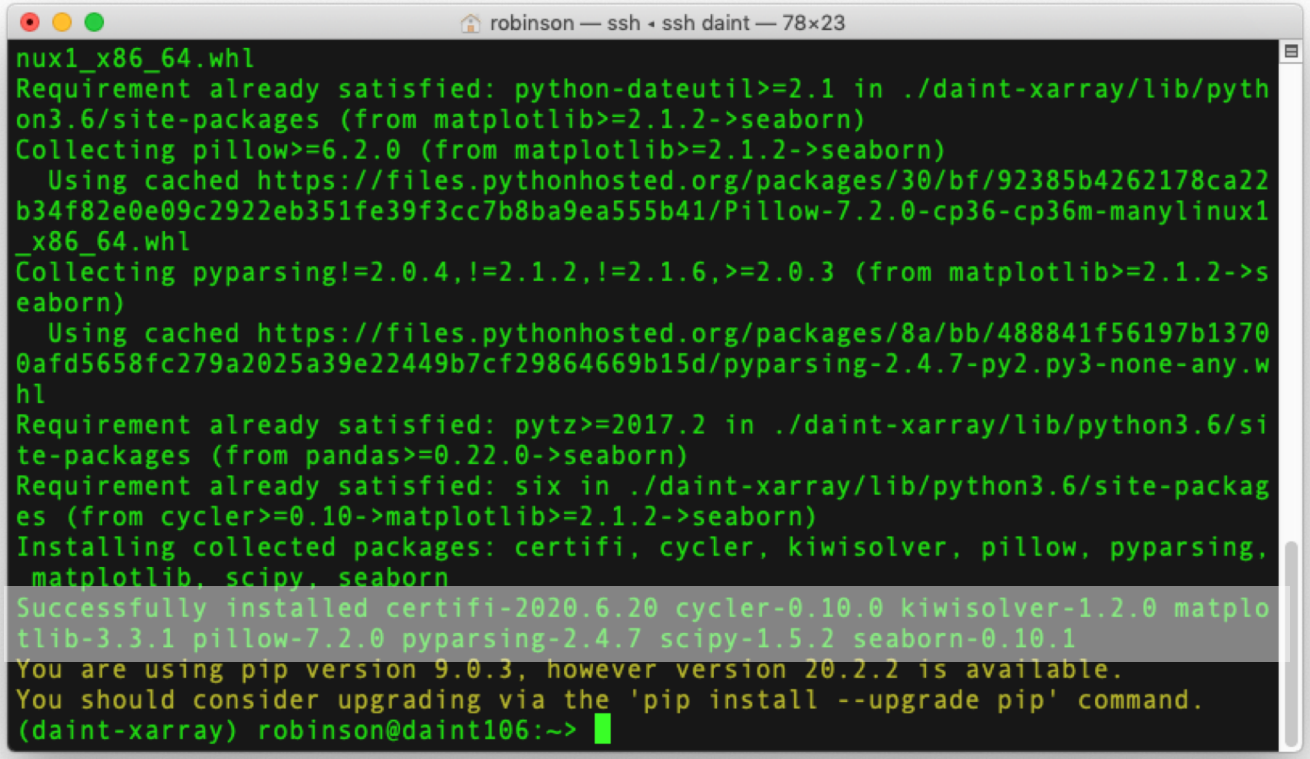

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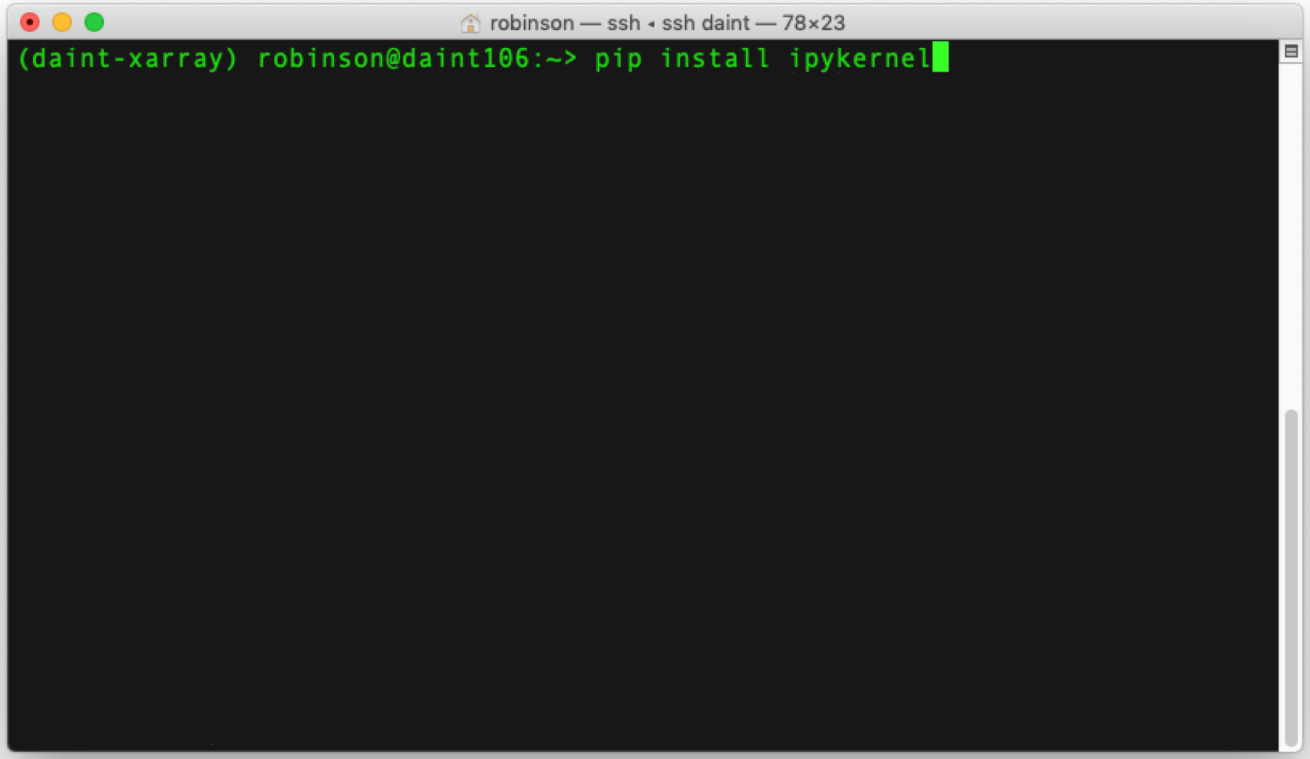

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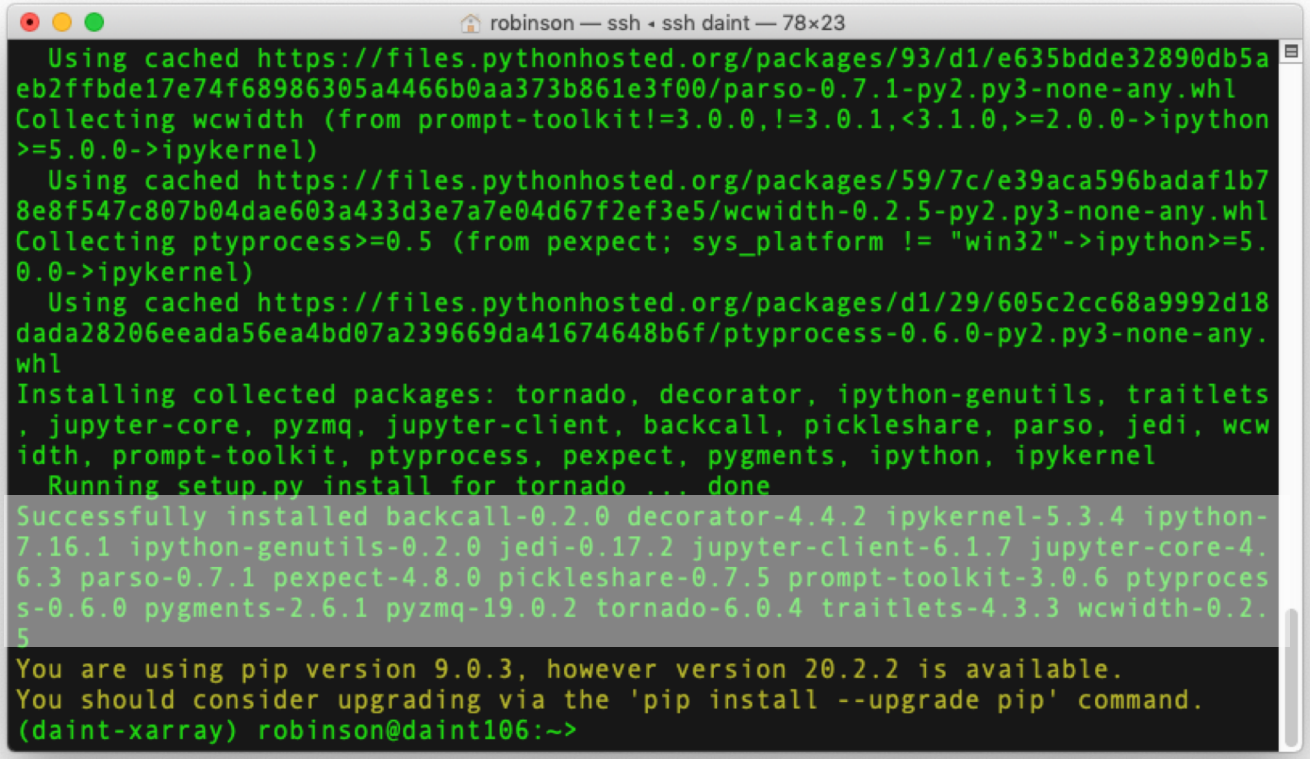

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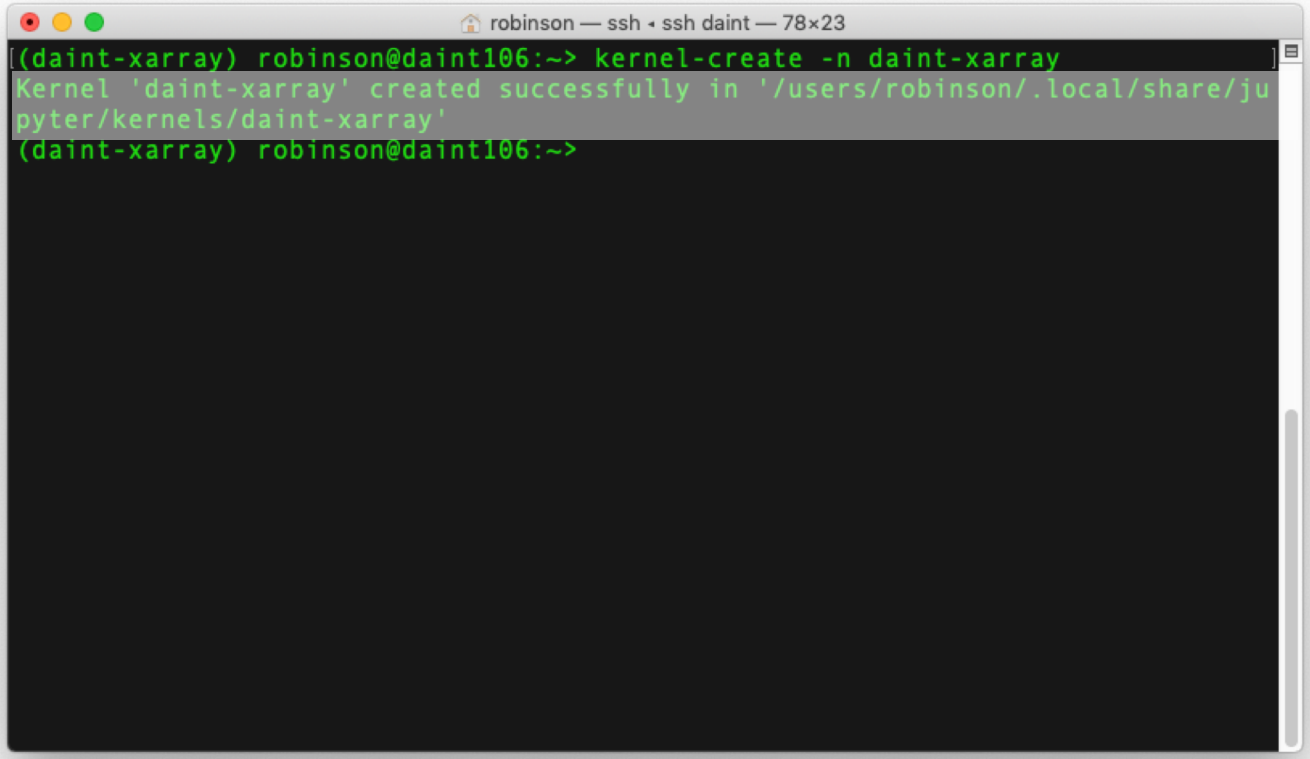
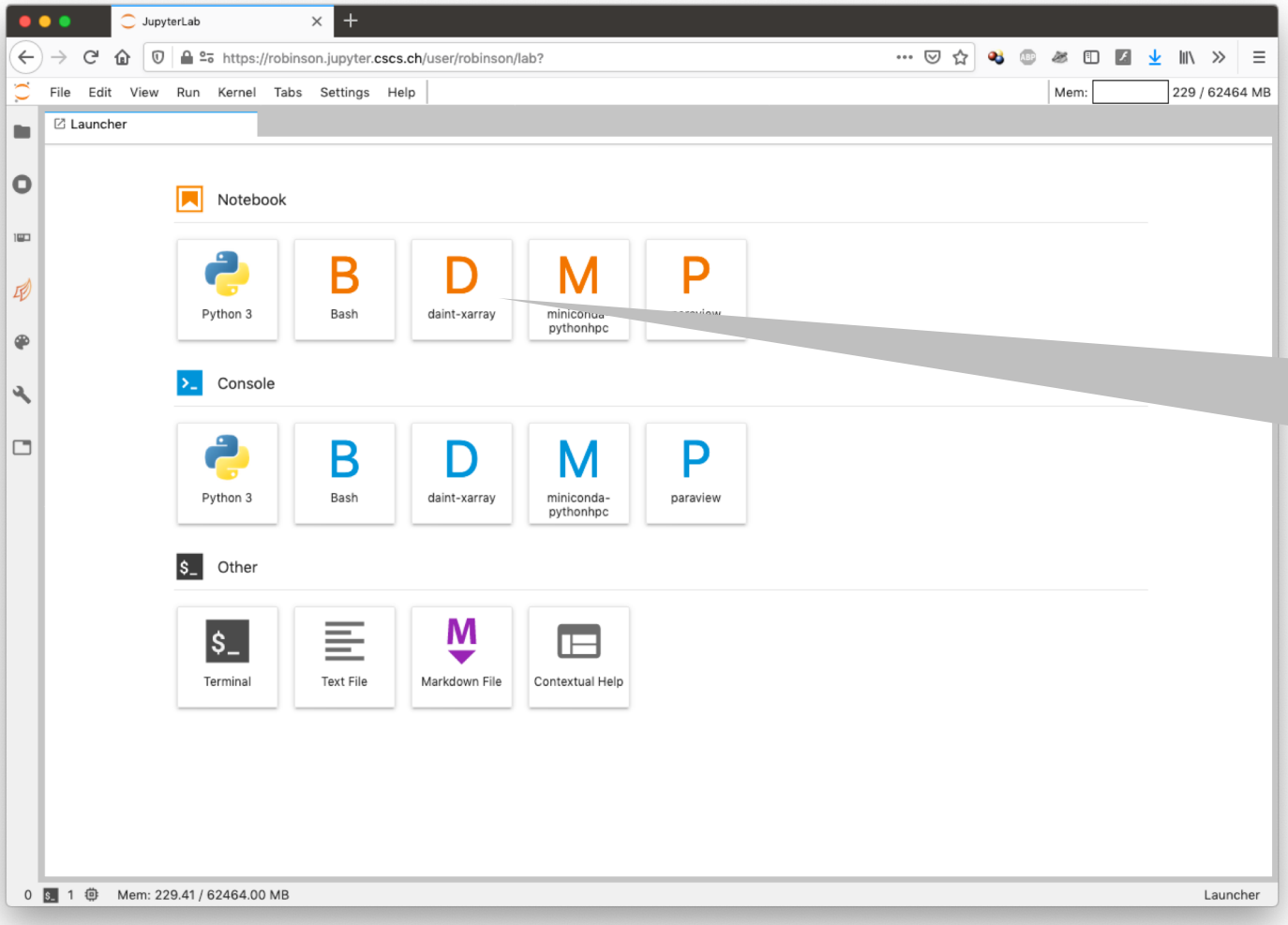
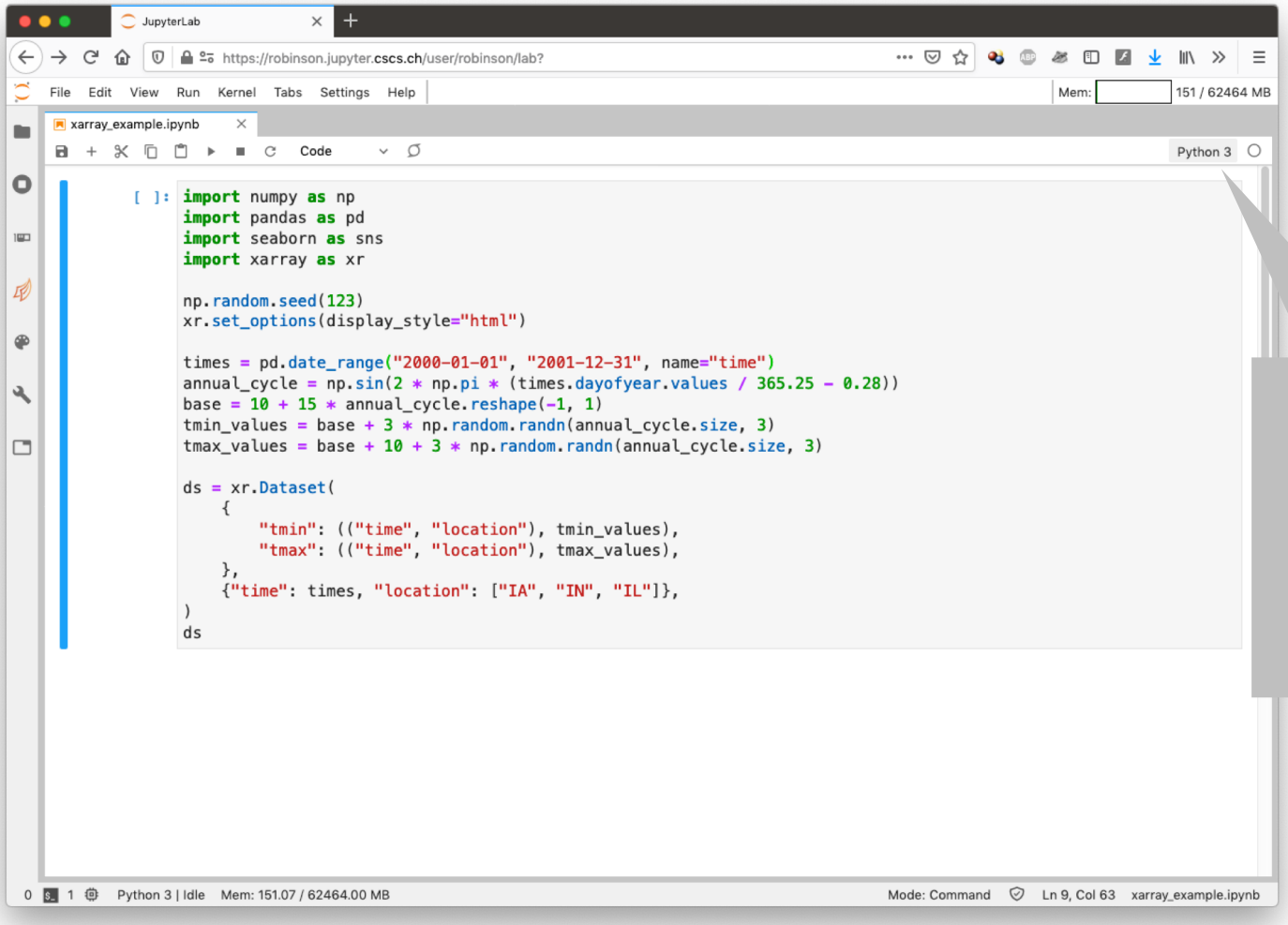


Using the new kernel

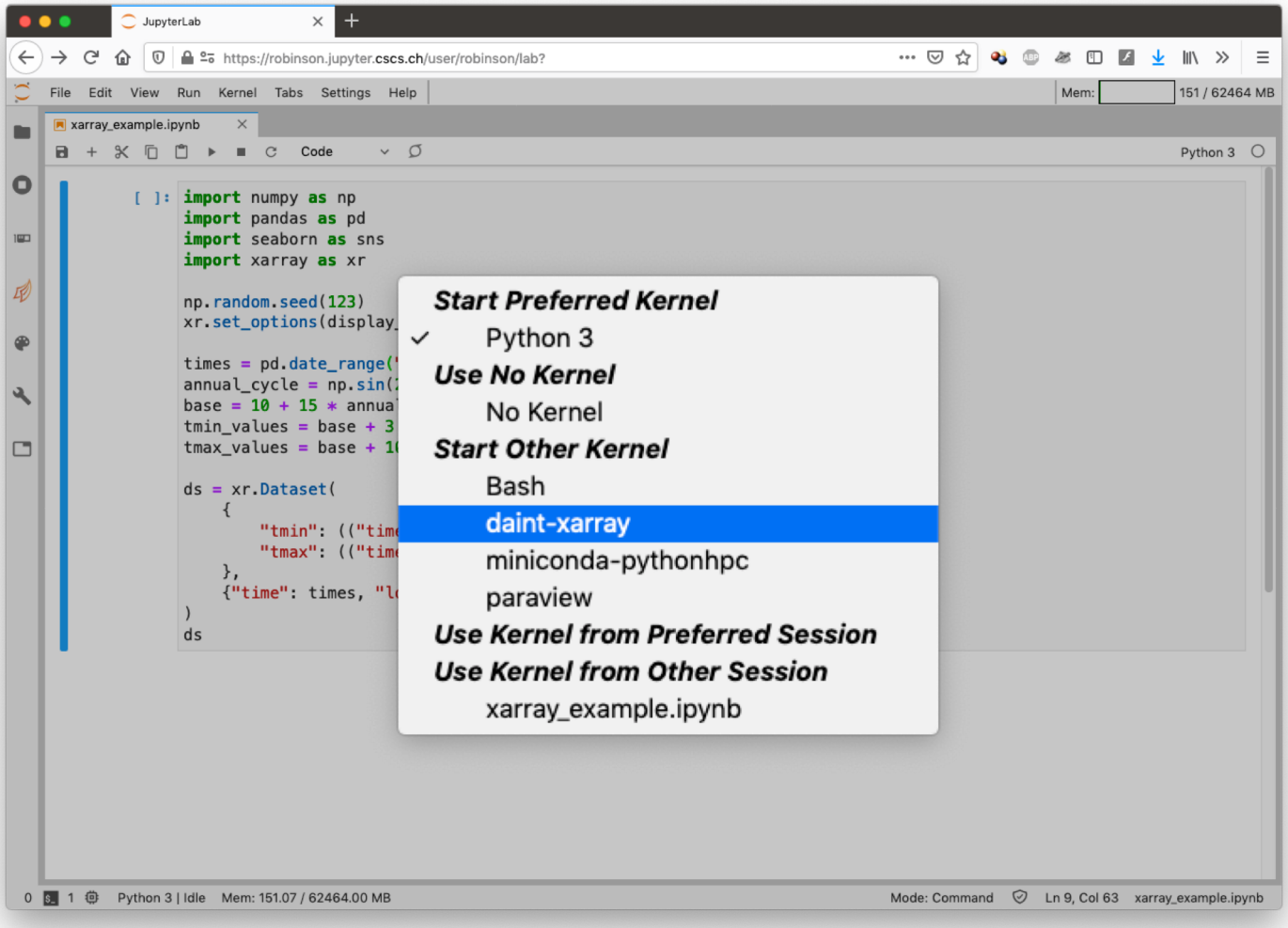


daint-xarray kernel will appear immediately

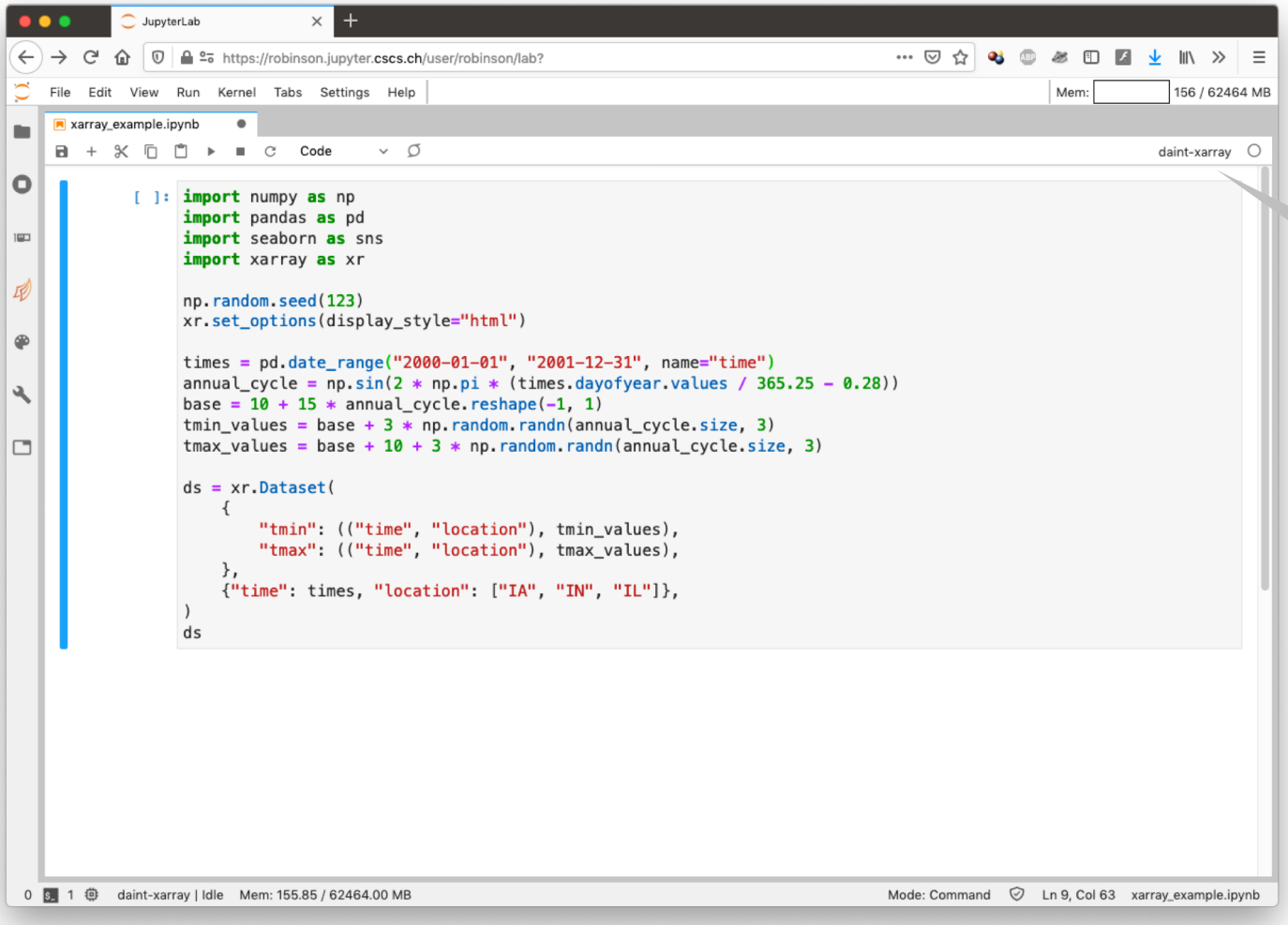
Using the new kernel



Using the new kernel

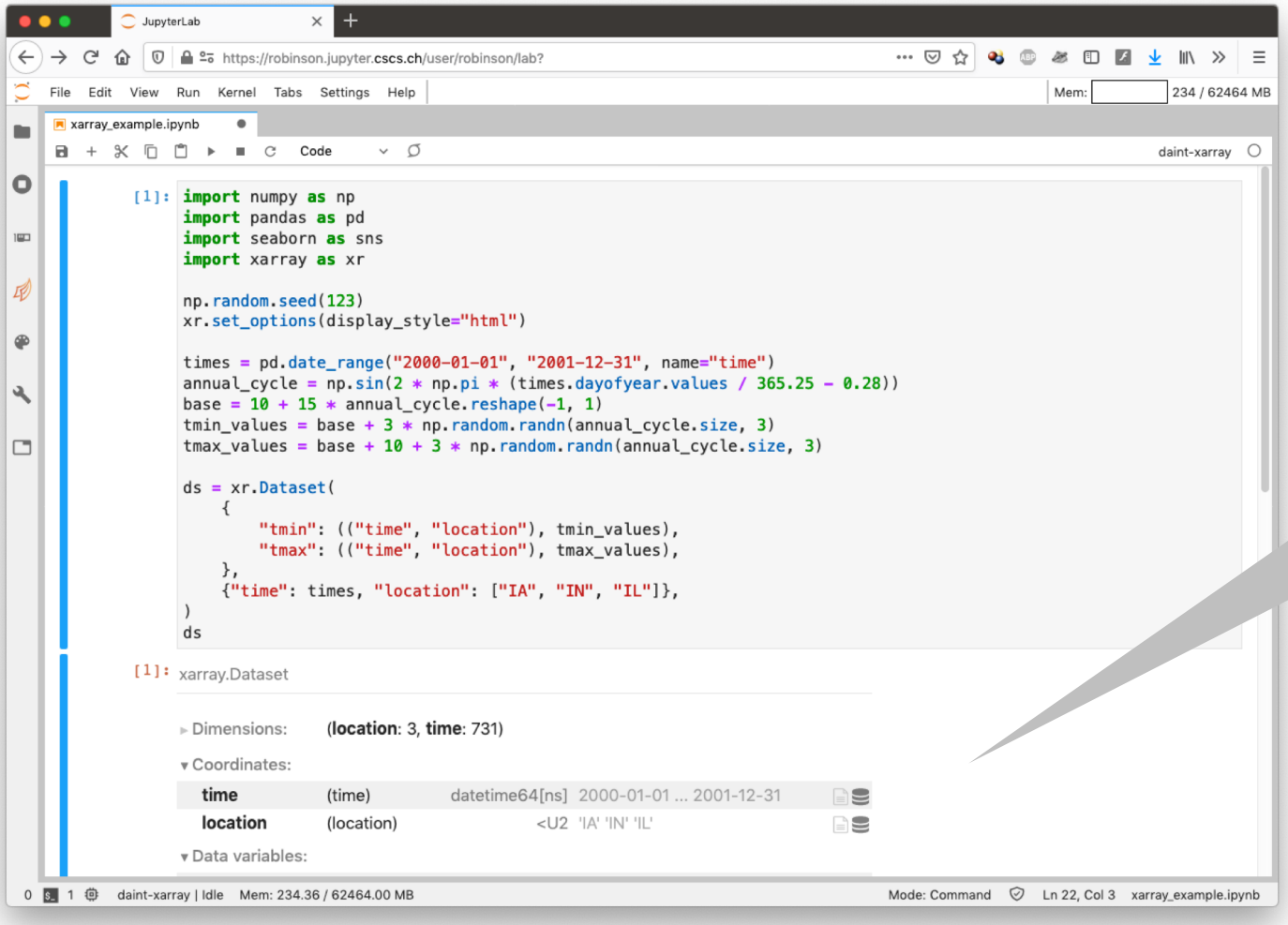


Using the new kernel



daint-xarray kernel

Using the new kernel



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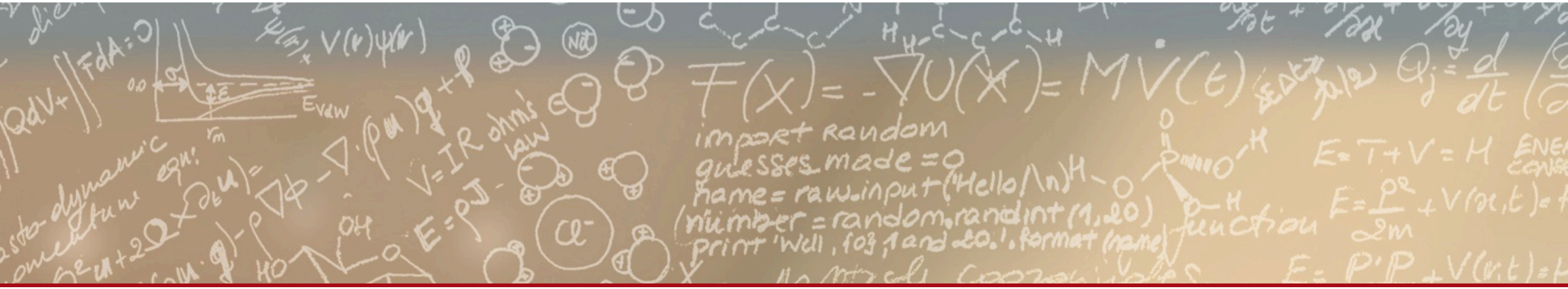

Have fun with Jupyter notebooks, and please let us know if you find the service useful.
We're interested in hearing about your use cases!

robinson@cscs.ch
help@cscs.ch