

MUSICA Tutorial Series 2021-2022: Getting started with JupyterHub

MUSICA: MULTI-Scale Infrastructure for Chemistry and Aerosols



12 November 2021



JupyterHub on cheyenne or casper at NCAR

See documentation on NCAR's Jupyterhub at:

<https://www2.cisl.ucar.edu/resources/jupyterhub-ncar>

To start a session, go to: <https://jupyterhub.hpc.ucar.edu/>



Select Production

You will need a login on cheyenne/casper to use this

Use your credentials to sign in



Online documentation for NCAR JupyterHub is available [here](#).

This development JupyterHub instance is subject to service interruptions on Tuesdays and Thursdays.

To avoid any inconvenience, please use [the stable instance](#).

Sign in

Username:

Password:

Sign in

Online documentation for NCAR JupyterHub is available [here](#).

Start My Server

Named Servers

In addition to your default server, you may have additional 4 server(s) with names. This allows you to have more than one server running at the same time.

Server name	URL	Last activity	Actions
<input type="text" value="Name your server"/>	Add New Server		
Example1		4 minutes ago	start delete

Click 'Start My Server'

Select Casper PBS batch or Cheyenne PBS batch

- You need to use casper to access campaign storage
- Using a batch node allows you to specify project number and memory

NCAR HPC JupyterHub

Cluster Selection

Casper PBS batch

Enter Queue or Reservation (-q)

casper

Specify your project account (-A)

Specify N node(s) (-l select=N)

1

Specify N CPUs per node (-l ncpus=N)

1

Specify N MPI tasks per node (-l mpirprocs=N)

1

Specify N threads per process (-l ompthreads=N)

1

Specify the Amount of memory / node in GB (MAX: 1494)

1

Specify X Number of GPUs / Node (-l ngpus=X)

0

Select GPU Type, X (-l gpu_type=X)

none

Specify wall time (-l walltime=[[HH:]MM:]SS) (24 Hr Maximum)

02:00:00

Launch Server

NCAR HPC JupyterHub

Cluster Selection

Casper login node

Casper login node

Casper PBS batch

Cheyenne login node

Cheyenne PBS batch

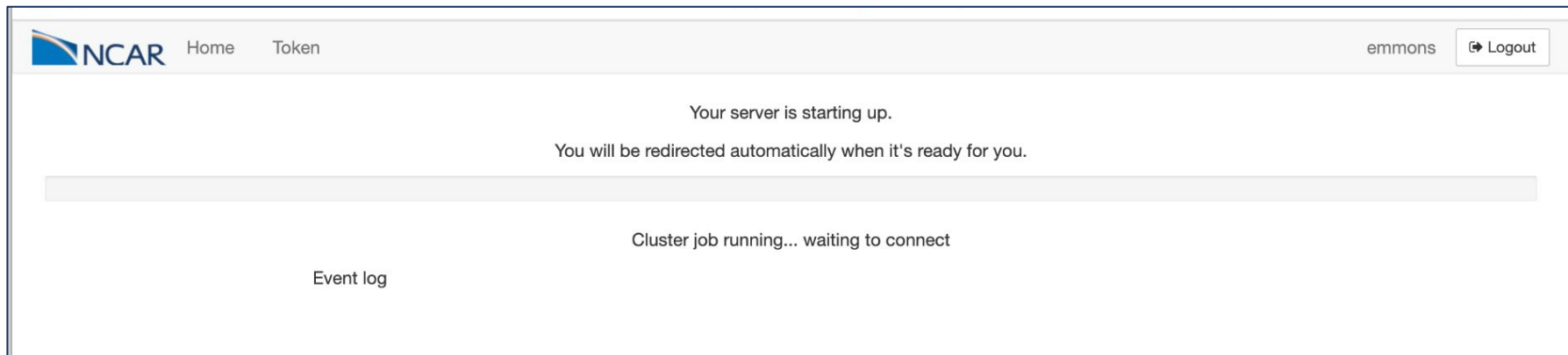
Enter your project number

You may need to increase memory, e.g. 5 GB

Increase walltime only if needed

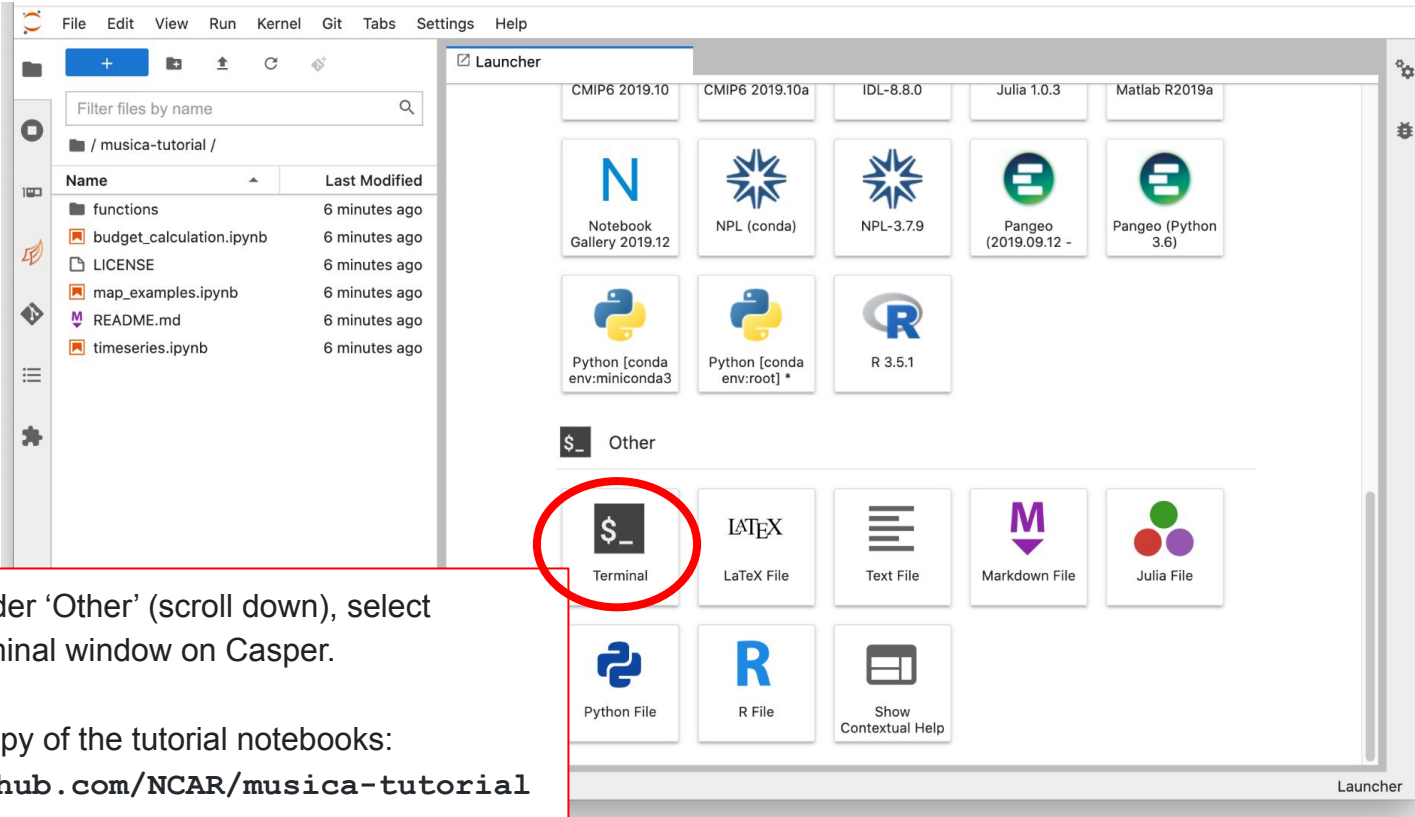
To reduce waiting time for Hub to start,
using smallest memory and walltime
possible

If the computer is busy you may need to wait for the server to connect....



If you have trouble connecting this way, you can try an alternate method:

https://ncar.github.io/CAM-chem/cheyenne_jupyter.html



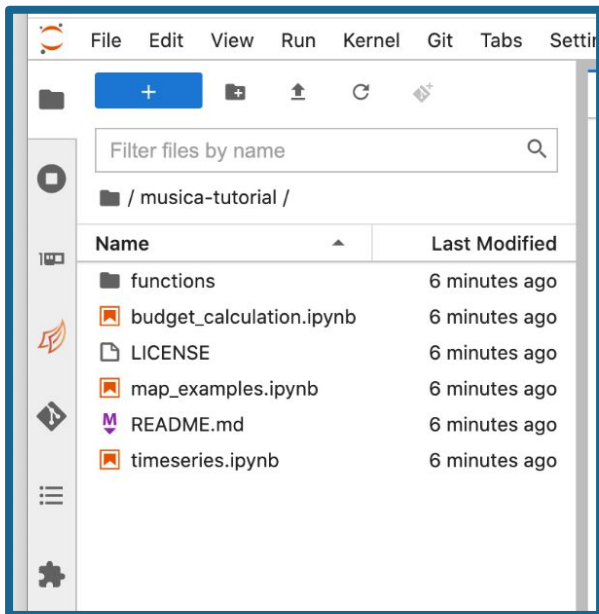
From the Launcher window, under 'Other' (scroll down), select 'Terminal'. This will open a terminal window on Casper.

In the terminal window, get a copy of the tutorial notebooks:

```
> git clone https://github.com/NCAR/musica-tutorial
```

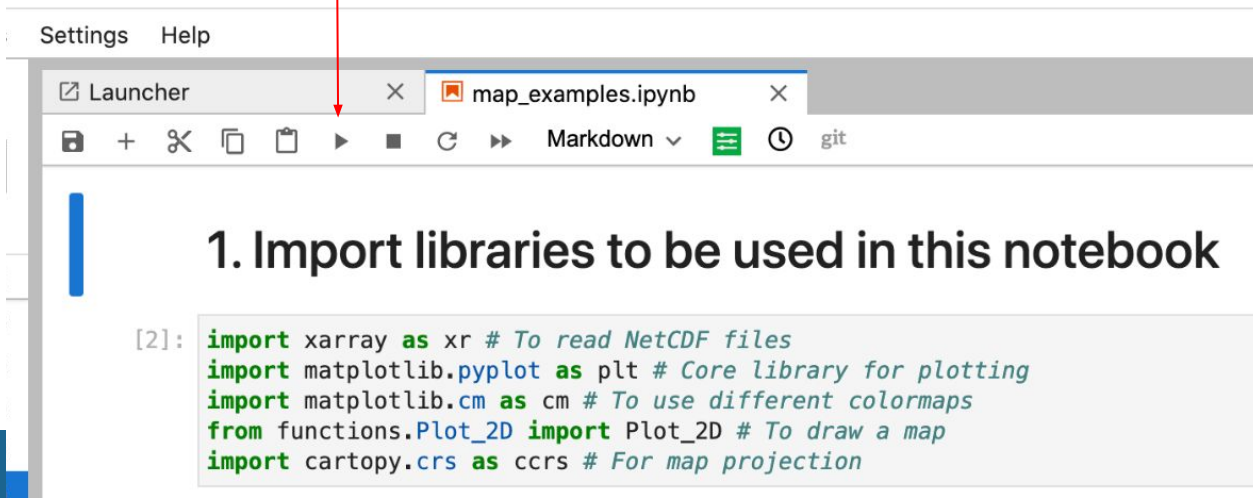
Navigate on the left panel to the new ***musica-tutorial*** directory to find the sample notebooks.

In the jupyter interface on the left side of the window navigate into this folder.



Open map_examples.ipynb

Click the play button to run each step of the notebook.
Wait until [*] at left of command switches to a number
before going on to next section. Creating plots may
take a few seconds.



When you open or create a new jupyter notebook file, you can select which kernel is used. We recommend using **NPL-3.7.9**.

When you are finished using JupyterHub, go to 'Hub Control Panel', under 'File' - this opens a new browser window. Click 'Stop My Server'. Then go back to original window and Log Out.

The map_examples notebook uses some standard python libraries, and the Plot_2D function (written by Duseong Jo, in your musica_tutorial/functions/ directory):

https://github.com/NCAR/CAM-chem/blob/main/docs_sphinx/examples/functions/Plot_2D.py

See more explanations of Plot_2D at:

<https://wiki.ucar.edu/display/MUSICA/Plot+output+with+Python>

Model output:

These tutorial examples read the MUSICA_{v0} Community Simulation for 2012-2013.

If you do not have a login on casper at NCAR, example files are available at:

ftp://[ftp.acom.ucar.edu/user/emmons/musica_tutorial_nov2021/](ftp://ftp.acom.ucar.edu/user/emmons/musica_tutorial_nov2021/)

The full dataset has just been published on the DASH Repository: <https://doi.org/10.5065/tgbj-yv18>

You can find out details of the content of these files by using ‘ncdump’ in the Terminal window in JupyterHub, e.g.:

```
> cd /glade/campaign/acom/acom-climate/tilmes/CO_CONUS/f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01/atm/hist  
> ncdump -h f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01.cam.h1.2013-08.nc  
> ncdump -h f.e22.FCcotagsNudged.ne0CONUSne30x8.cesm220.2012-01.cam.h1.2013-08.nc | grep O3
```

The tutorial notebooks also show how to find this information with python within the notebook.

More Tips:

- If you start reaching your memory limit (shown at the bottom of the Hub window), try restarting the kernel (find under the Kernel menu, or the circle with arrow symbol in the toolbar).
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