

# MUSICA Tutorial: Getting started with JupyterHub

**MUSICA: MULTI-Scale Infrastructure for Chemistry and Aerosols**



20 Sep 2024



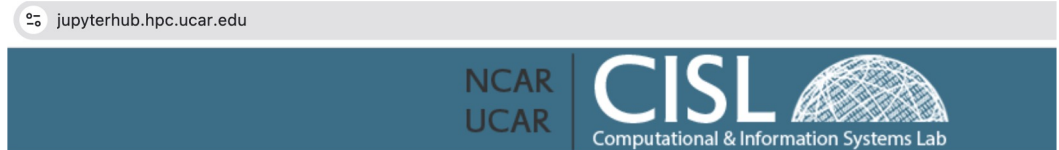
# JupyterHub on cheyenne or casper at NCAR

See documentation on NCAR's Jupyterhub at: <https://ncar-hpc-docs.readthedocs.io/en/latest/compute-systems/jupyterhub/>

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

You will need a login on NCAR HPC (derecho, casper) to use this

**1. Select  
Production**



**Available NCAR Resources**

*Production*

## 2. Use your username, password and DUO push to login



Sign in

**Username:**

**Password:**

Sign in

### 3. Select start

[Home](#)[Token](#)[NCAR ▾](#)

jzhan166

[Logout](#)

Server name	Resource	Last activity	Time Remaining	Actions
<input type="text" value="Name your server"/>	<a href="#">Add New Server</a>			
Default		2024-09-15 20:40 UTC	-	<a href="#">start</a>

## 4. Select Casper PBS Batch



Home

Token

NCAR ▾

jzhan166

Logou

# NCAR HPC JupyterHub

Casper PBS Batch

✓ Casper Login

Derecho

Launch Server

**Click 'Start My Server'**

## 5. change your settings

### NCAR HPC JupyterHub

**Resource Selection**

Casper PBS Batch

**Queue or Reservation (-q)**

casper

**Project Account (-A)**

NACD0028

**Specify N Nodes (-l select=N)**

1

**Specify N CPUs per Node (-l ncpus=N)**

1

**Specify Threads per Process (-l ompthreads=N)**

1

**Specify MPI processes per Node (-l mpirprocs=N)**

1

**Specify Memory per Node in GB (-l mem=N)**

4

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

0

**Select GPU Type, X (-l gpu\_type=X)**

none

**Wall Time HH:MM:SS (24-hour max)**

02:00:00

**Jupyter Environment**

Base

Launch Server

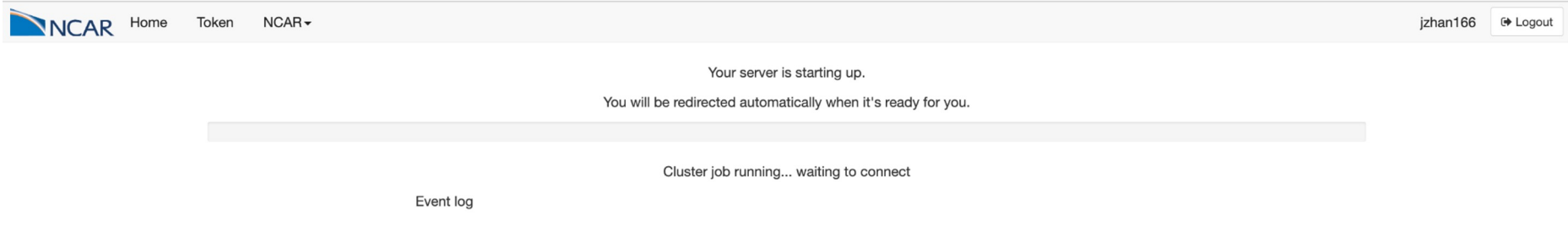
**Select your project number  
(NACD0028)**

**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....



The screenshot shows a web interface with a header bar. On the left, there is a logo for NCAR and navigation links for Home, Token, and NCAR with a dropdown arrow. On the right, the user is logged in as 'jzhan166' and there is a Logout button. The main content area displays a message: 'Your server is starting up. You will be redirected automatically when it's ready for you.' Below this message is a long, thin grey progress bar. At the bottom of the message area, it says 'Cluster job running... waiting to connect'. There is also a link labeled 'Event log' on the left side of the page.

NCAR Home Token NCAR ▾

jzhan166 Logout

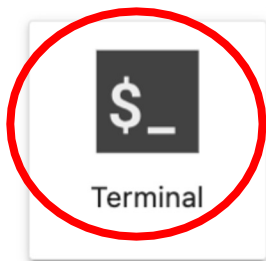
Your server is starting up.  
You will be redirected automatically when it's ready for you.

Cluster job running... waiting to connect

Event log

## 6. open terminal (under Other) This will open a terminal window on Casper.

\$ \_ Other



Terminal



Text File

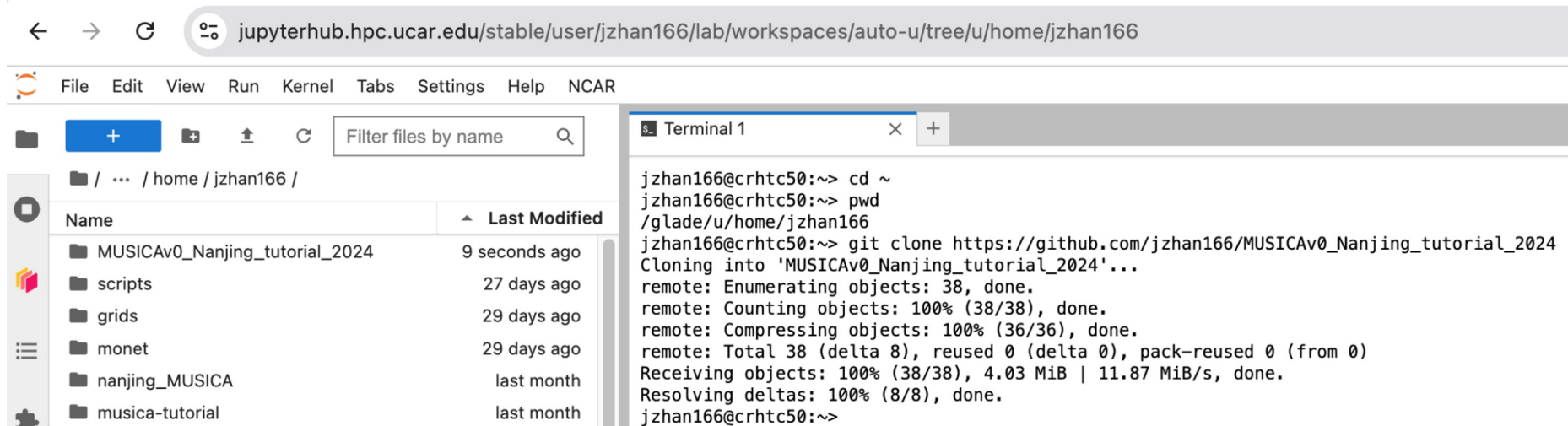
In the terminal window

Type:

`cd ~`

then type:

`git clone https://github.com/jzhan166/MUSICAv0\_Nanjing\_tutorial\_2024`



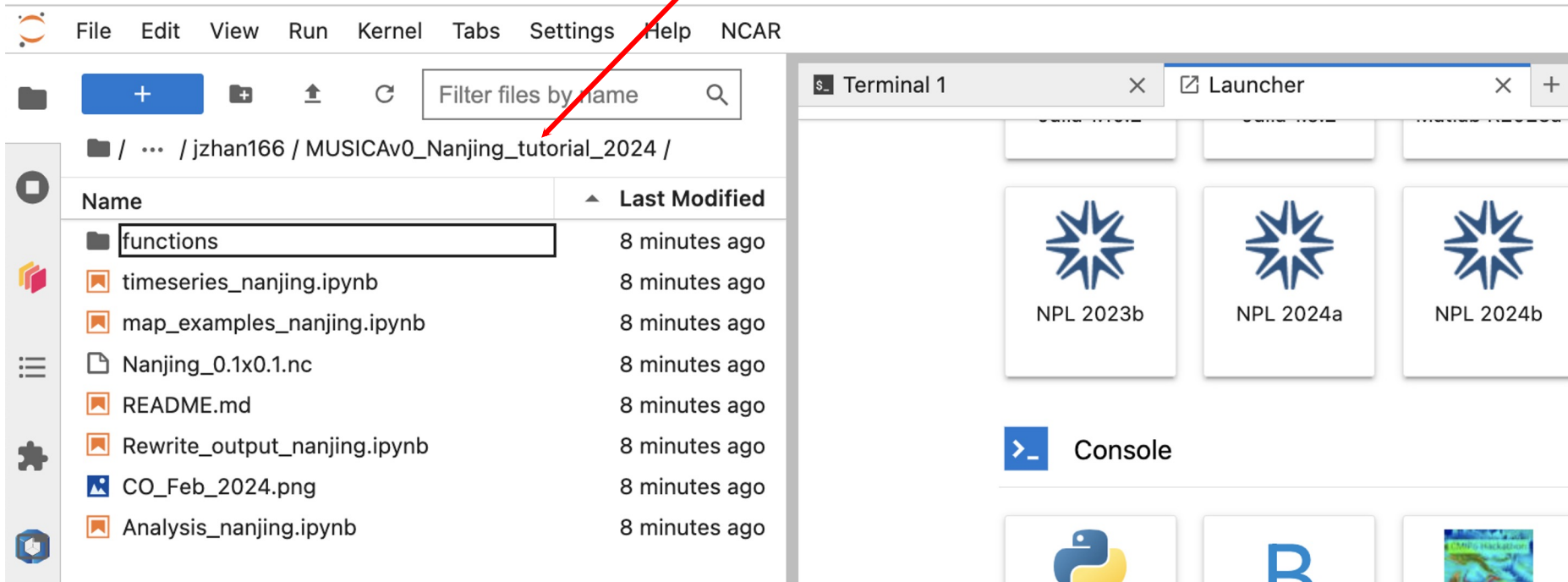
The screenshot shows a JupyterLab interface. The browser address bar displays `jupyterhub.hpc.ucar.edu/stable/user/jzhan166/lab/workspaces/auto-u/tree/u/home/jzhan166`. The top menu bar includes File, Edit, View, Run, Kernel, Tabs, Settings, Help, and NCAR. The left sidebar shows a file browser with a search bar and a list of files and folders. The main area displays a terminal window titled "Terminal 1" with the following output:

```
jzhan166@crhtc50:~> cd ~
jzhan166@crhtc50:~> pwd
/glade/u/home/jzhan166
jzhan166@crhtc50:~> git clone https://github.com/jzhan166/MUSICAv0_Nanjing_tutorial_2024
Cloning into 'MUSICAv0_Nanjing_tutorial_2024'...
remote: Enumerating objects: 38, done.
remote: Counting objects: 100% (38/38), done.
remote: Compressing objects: 100% (36/36), done.
remote: Total 38 (delta 8), reused 0 (delta 0), pack-reused 0 (from 0)
Receiving objects: 100% (38/38), 4.03 MiB | 11.87 MiB/s, done.
Resolving deltas: 100% (8/8), done.
jzhan166@crhtc50:~>
```

Name	Last Modified
MUSICAv0_Nanjing_tutorial_2024	9 seconds ago
scripts	27 days ago
grids	29 days ago
monet	29 days ago
nanjing_MUSICA	last month
musica-tutorial	last month



7. Navigate on the left panel to the new **MUSICAv0\_Nanjing\_tutorial\_2024** directory to find the sample notebooks.



The screenshot displays the NCAR JupyterLab interface. The top menu bar includes File, Edit, View, Run, Kernel, Tabs, Settings, Help, and NCAR. The left sidebar shows a file browser with the path `/ ... / jzhan166 / MUSICAv0_Nanjing_tutorial_2024 /`. A search bar is labeled "Filter files by name". The file list is as follows:

Name	Last Modified
functions	8 minutes ago
timeseries_nanjing.ipynb	8 minutes ago
map_examples_nanjing.ipynb	8 minutes ago
Nanjing_0.1x0.1.nc	8 minutes ago
README.md	8 minutes ago
Rewrite_output_nanjing.ipynb	8 minutes ago
CO_Feb_2024.png	8 minutes ago
Analysis_nanjing.ipynb	8 minutes ago

The right sidebar contains a "Launcher" panel with three NPL icons labeled "NPL 2023b", "NPL 2024a", and "NPL 2024b". Below the launcher is a "Console" panel with a prompt `>_`. At the bottom, there are icons for Python, R, and a map.

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

Open **map\_examples\_nanjing.ipynb**

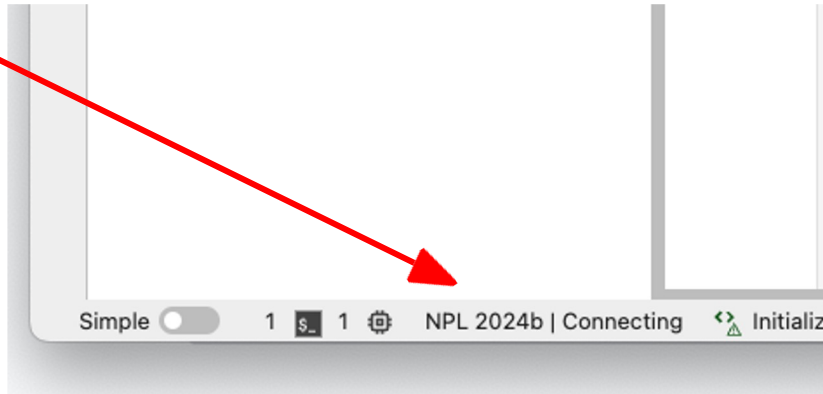
Click the play button to run each step of the notebook.

Wait until [\*] at left of command switches to a number before going on to next section. Creating plots may take a few seconds.

The screenshot shows the JupyterLab interface. On the left is a file browser with a table of files and folders. The file 'map\_examples\_nanjing.ipynb' is selected. On the right is a notebook with a terminal window at the top and a code cell below. The code cell contains the following code:

```
[1]: import numpy as np # for array manipulation and basic scientific calculation
import xarray as xr # To read NetCDF files
import matplotlib.pyplot as plt # Core library for plotting
import matplotlib.cm as cm # To use different colormaps
from functions.Plot_2D import Plot_2D # To draw a map
import cartopy.crs as ccrs # For map projection
```

When you open or create a new jupyter notebook file, you can select which kernel is used (lower left corner). We recommend using **NPL 2024a or 2024b**.



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](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:

```
/glade/campaign/acom/acom-weather/emmons/tutorial_nanjing/f.e3beta01.FCnudged.Nanjing_ne30x8.02/atm/hist/
```

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-weather/emmons/tutorial_nanjing/f.e3beta01.FCnudged.Nanjing_ne30x8.02/atm/hist/
```

```
ncdump -h f.e3beta01.FCnudged.Nanjing_ne30x8.02.cam.h0a.2024-01.nc
```

```
ncdump -h f.e3beta01.FCnudged.Nanjing_ne30x8.02.cam.h0a.2024-01.nc | grep O3
```

## 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).
- 

