MUSICA Tutorial Series 2021-2022: Introduction to MELODIES-MONET

MUSICA: MUlti-Scale Infrastructure for Chemistry and Aerosols

NCAR

11 March 2022

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MELODIES: Model EvaLuation using Observations, DIagnostics and Experiments Software

MONET: Model and ObservatioN Evaluation Toolkit

Current developers:

Rebecca Buchholz, David Fillmore, Duseong Jo, Louisa Emmons - NCAR/ACOM

Becky Schwantes, **Barry Baker**, Zachary Moon, Maggie Bruckner, Meng Li, Jian He, et al. – NOAA (CSL, GSL, ARL)

A modular framework to compare model results and observations of atmospheric chemistry

In Python, using Xarray, NumPy, SciPy, Pandas, …

Goal: to be able to read any model and pair it to observations (surface in situ and remote sensing, aircraft, satellite, …)

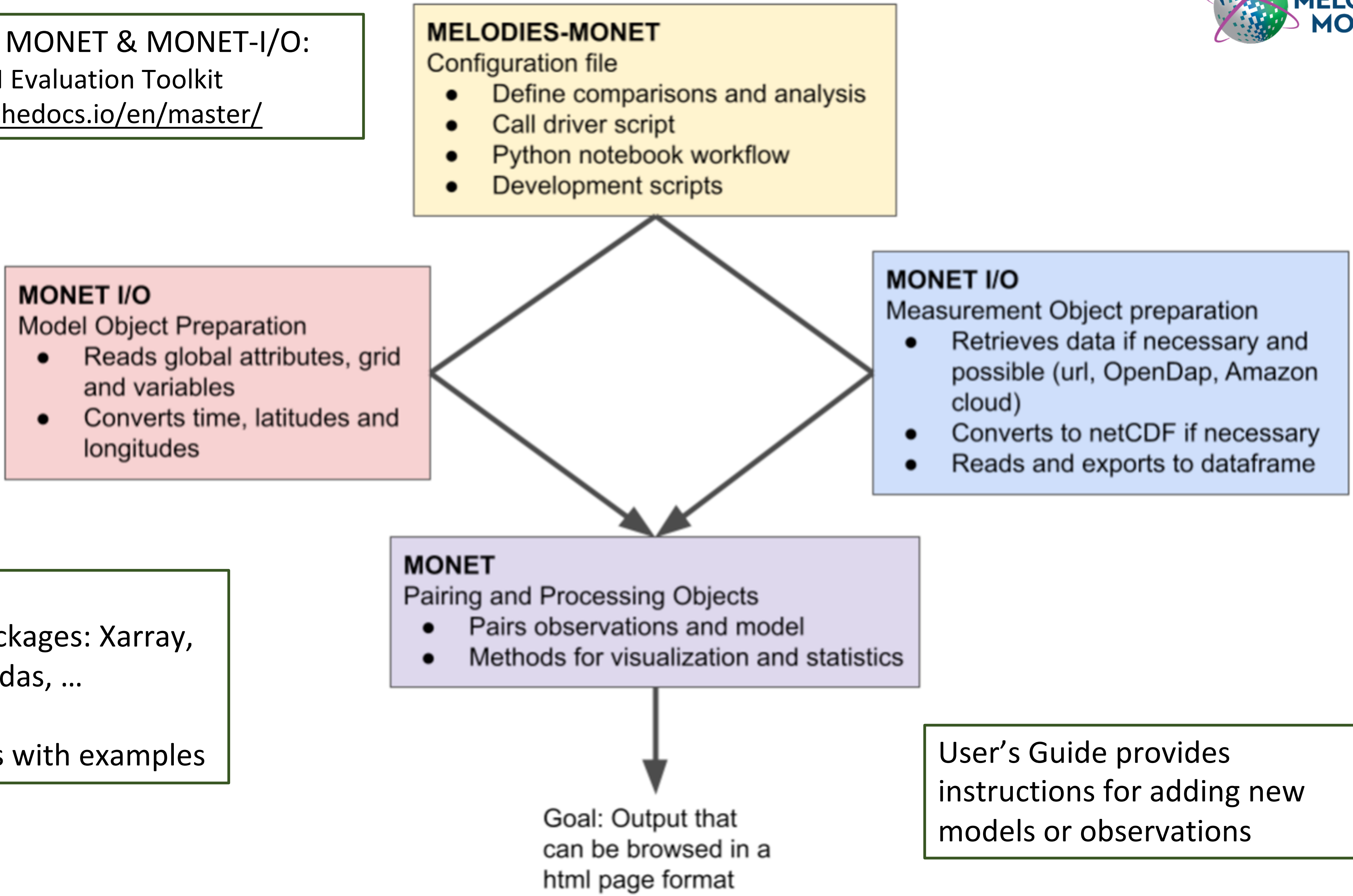
EarthCube

NOAA

NCAR
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

Warning: Still under development!

MELODIES is built on MONET & MONET-I/O:
Model and ObservatioN Evaluation Toolkit
https://monet-arl.readthedocs.io/en/master/



Written in Python
Using standard packages: Xarray, NumPy, SciPy, Pandas, …

Jupyter Notebooks with examples

User's Guide provides instructions for adding new models or observations

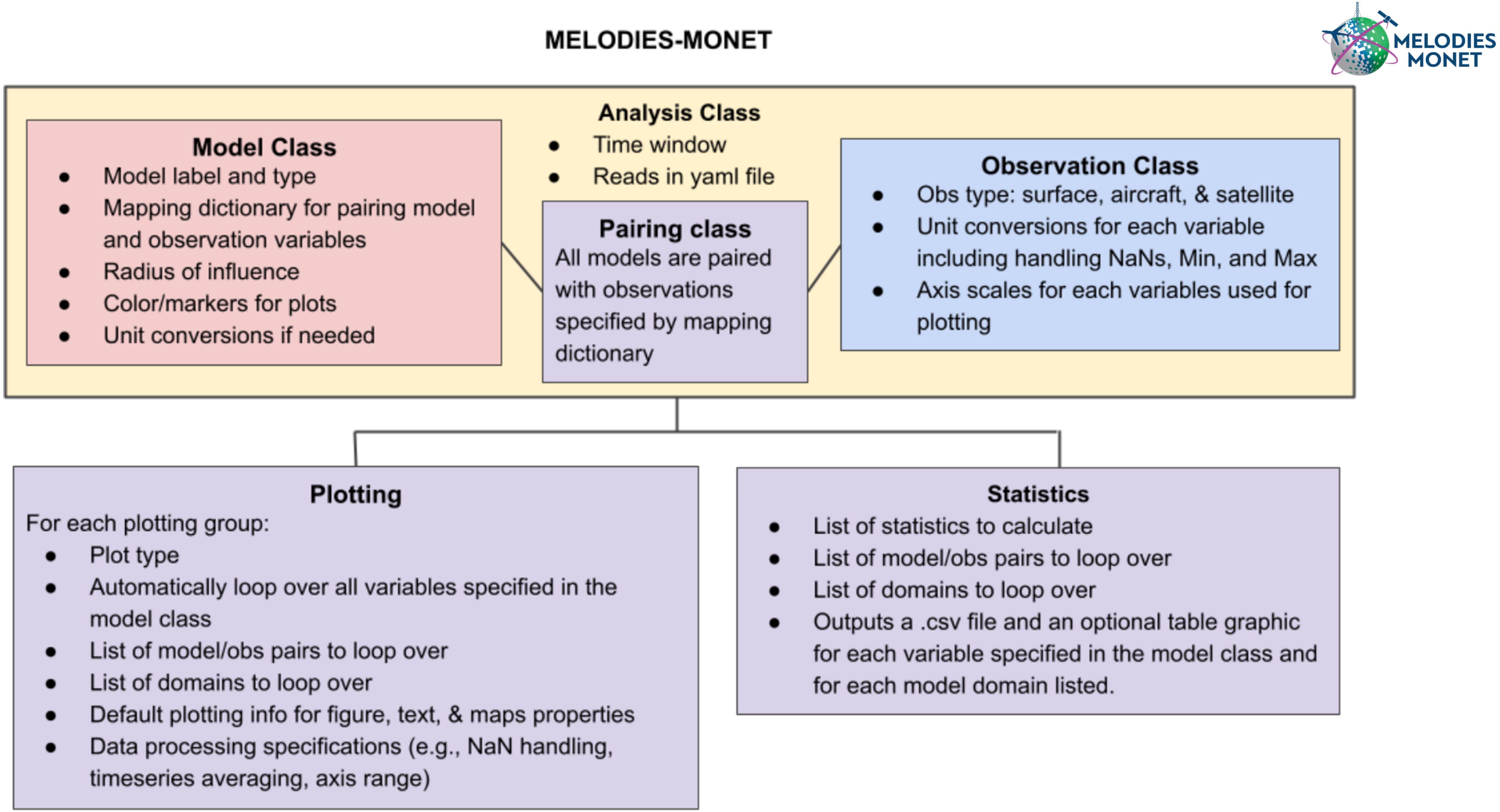


Fig. 1: Schematic of the classes defined in the Python code and used by MELODIES MONET.

MELODIES-MONET Driver:

1. Reads in the yaml file
2. Reads in the model results
3. Reads in the observations
4. Pairs the model and observations and stores them as class “pair”
5. Then the plotting routines reads this class “pair” and calls general plotting routines to make the plots, with options such as:
   Calculate regulatory metrics (PM2.5 daily average, and MDA8 ozone)
   Separate by region (depending on categories available in dataset)

For each of the observations, unit conversions will be applied.

- Gases are all in ppbv and aerosols in ug/m3
- others like meteorology are not as standardized yet

MELODIES-MONET: https://github.com/NOAA-CSL/MELODIES-MONET
Documentation: https://melodies-monet.readthedocs.io/

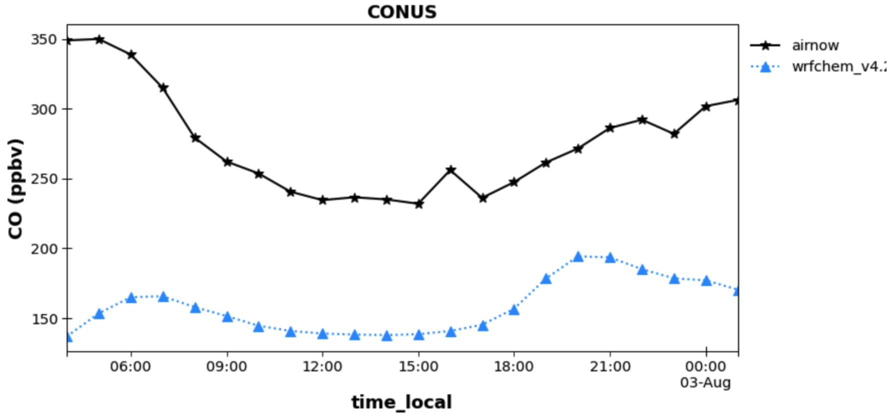
In [11]:

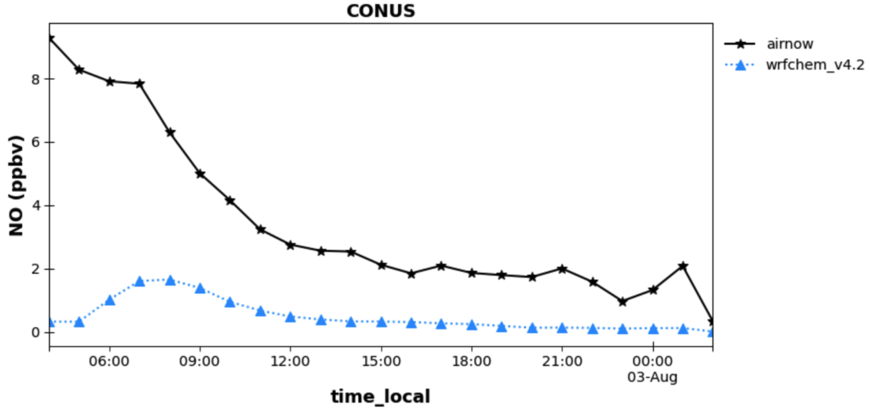
```python
#This just pairs the data
an.pair_data()
```

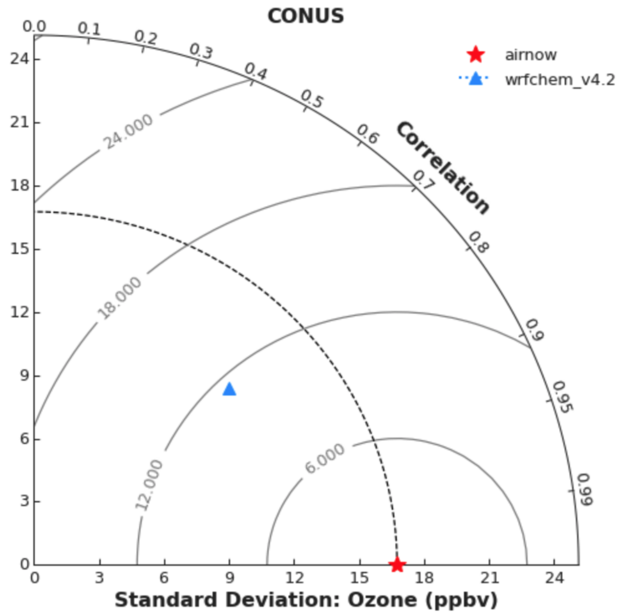
```
[########################################] | 100% Completed |  0.1s
[########################################] | 100% Completed |  0.1s
[########################################] | 100% Completed |  0.2s
[########################################] | 100% Completed |  0.2s
```

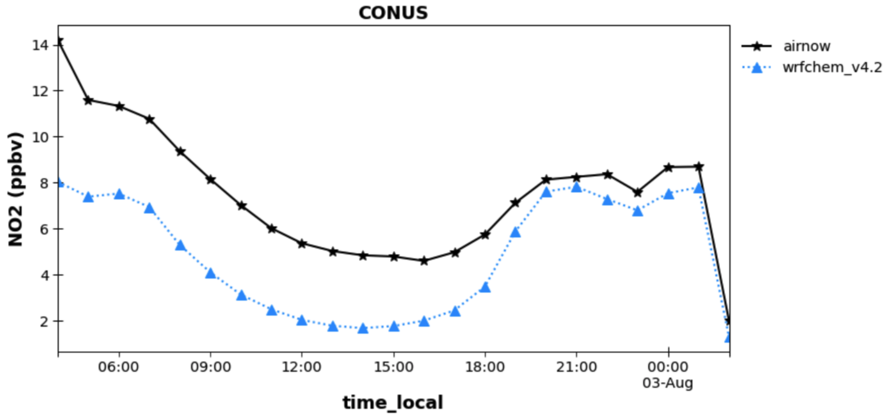
In [12]:

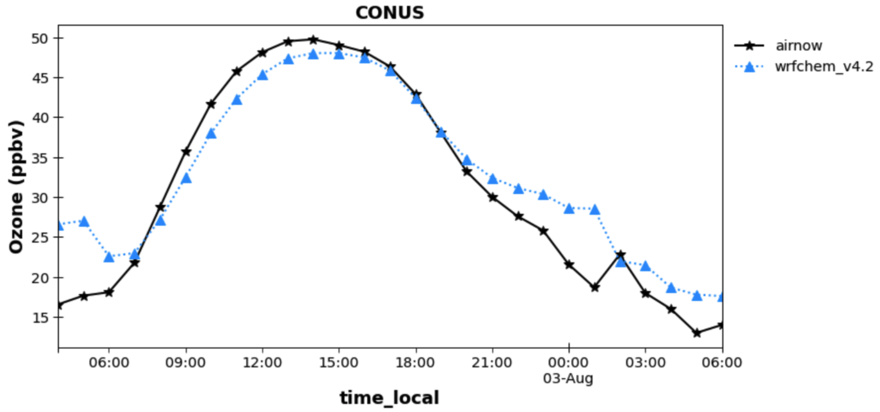
```python
#And this generates all the plots.
an.plotting()
```

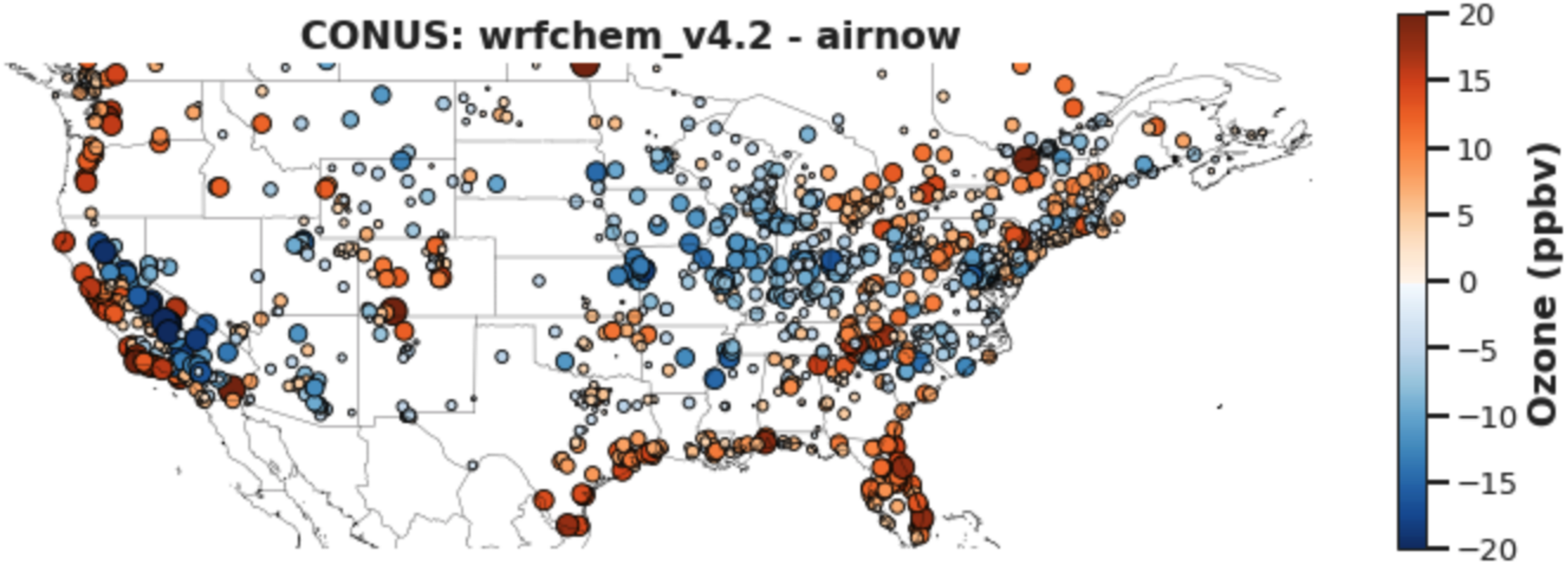


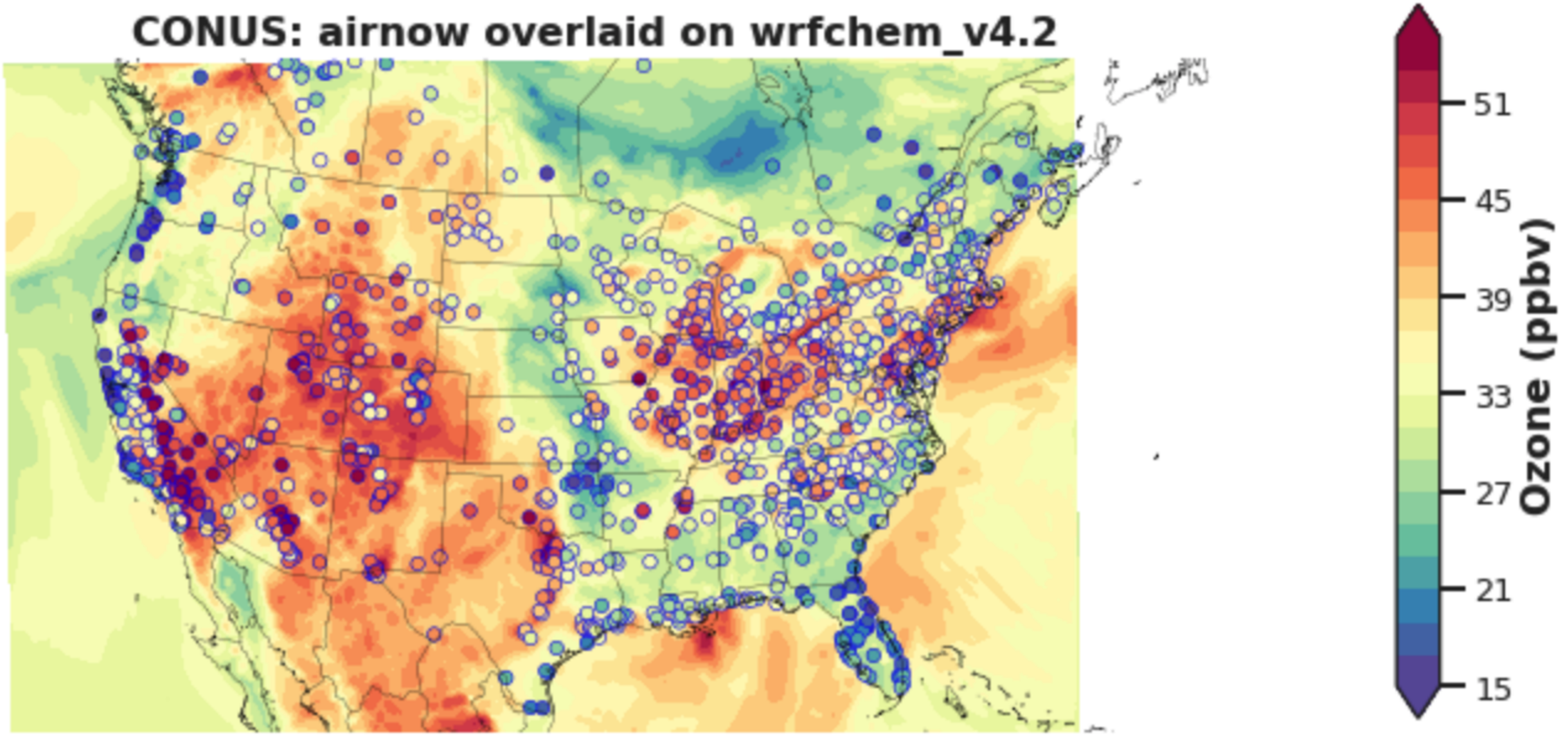


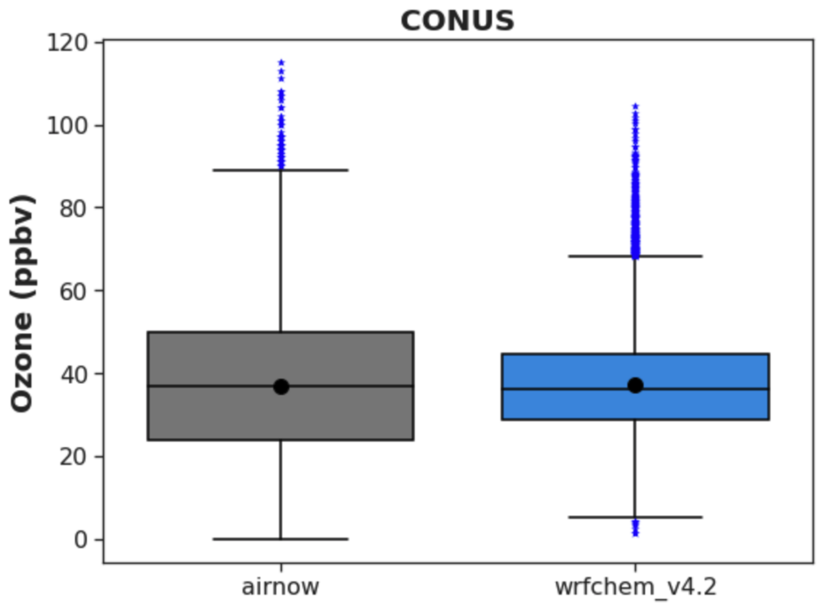












MELODIES MONET

Examples of Output: Statistics

August 2019 - Average in WRF-chem

Statistics of OZONE and o3 pair over file period 2019-08-01_06 to 2019-09-01_05

Number of OZONE Observations = 39986
Number of o3 Predictions = 39986
Number of OZONE/o3 Observations/Prediction Pairs (#) = 39986
Mean of OZONE Observations = 42.82
Mean of o3 Predictions = 46.30
Median of OZONE Observations = 42.50
Median of o3 Predictions = 44.86
Standard deviation of OZONE Observations = 12.91
Standard deviation of o3 Predictions = 11.43
Mean Bias of o3-OZONE = 3.48
Normalized Mean Bias (%) of o3-OZONE = 8.13
Normalized Mean Error (%) of o3-OZONE = 16.74
Root Mean Square Error of o3-OZONE = 9.26
Index of Agreement of o3-OZONE = 0.85
Pearsons Correlation Coefficient of o3-OZONE = 0.76

Statistics of PM2.5 and PM25 pair over file period 2019-08-01_06 to 2019-09-01_05

Number of PM2.5 Observations = 27981
Number of PM25 Predictions = 27981
Number of PM2.5/PM25 Observations/Prediction Pairs (#) = 27981
Mean of PM2.5 Observations = 7.06
Mean of PM25 Predictions = 9.87
Median of PM2.5 Observations = 6.50
Median of PM25 Predictions = 8.09
Standard deviation of PM2.5 Observations = 3.25
Standard deviation of PM25 Predictions = 6.43
Mean Bias of PM25-PM2.5 = 2.82
Normalized Mean Bias (%) of PM25-PM2.5 = 39.91
Normalized Mean Error (%) of PM25-PM2.5 = 67.45
Root Mean Square Error of PM25-PM2.5 = 6.63
Index of Agreement of PM25-PM2.5 = 0.49
Pearsons Correlation Coefficient of PM25-PM2.5 = 0.38

Development plans

Short-term, in progress:

- Reading aircraft campaign observations
- Reading satellite retrievals, applying averaging kernels, for swaths & gridded
- Reading additional models

Longer-term goals:

- MELODIES-Climate – same structure as MELODIES-MONET but would compare model(s) to climatologies of observations
- Connect with METPLUS
    - Have METPlus call MELODIES-MONET
    - Take advantage of MET statistics and plotting
    - METplus will use MONET I/O

Please get involved and contribute!

MELODIES MONET is a community-driven project.

We welcome collaborations and contributions.

- Ask questions, suggest features, or view source code on GitHub: https://github.com/NOAA-CSL/MELODIES-MONET
- If an issue arises, please post on GitHub Issues: https://github.com/NOAA-CSL/MELODIES-MONET/issues
- Please check out GitHub Projects: https://github.com/NOAA-CSL/MELODIES-MONET/projects to learn about current development plans

Installation of MELODIES-MONET

Please find instructions specific for this tutorial in this doc:

https://bit.ly/melodies-tutorial

General installation instructions are in the MELODIES-MONET documentation:

https://melodies-monet.readthedocs.io/en/develop/tutorial/installation.html

As the code is currently in a state of rapid development, please check the melodies-monet site for the latest instructions

Hands-on examples

- Minimal example (WRF-Chem vs AIRNOW) - David Fillmore (NCAR)
- Idealized example - Zachary Moon (NOAA)
- Using MUSICA (variable unstructured model grid) - Duseong Jo (NCAR)
- Comparing multiple models (Taylor diagram) - Rebecca Buchholz (NCAR)

End of presentation - switch to JupyterHub notebooks

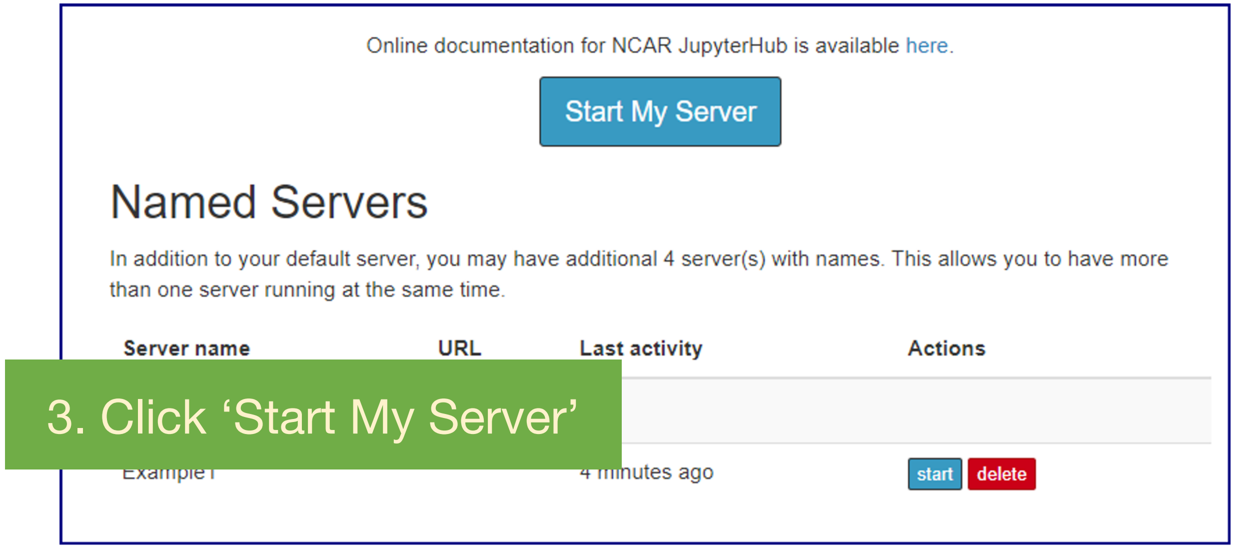
The following slide provide some instructions and tips for getting started on NCAR's JupyterHub system and starting the example notebooks.

1. Start NCAR JupyterHub: https://jupyterhub.hpc.ucar.edu/
(you must have an account on cheyenne/casper)

If you need more information see:
https://arc.ucar.edu/knowledge_base/70549913#JupyterHubatNCAR-Gettingstarted

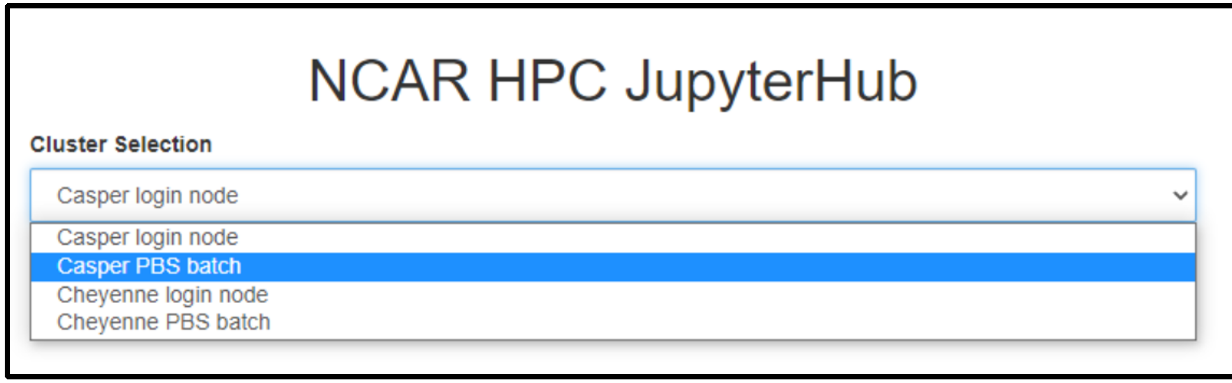
2. Select Production

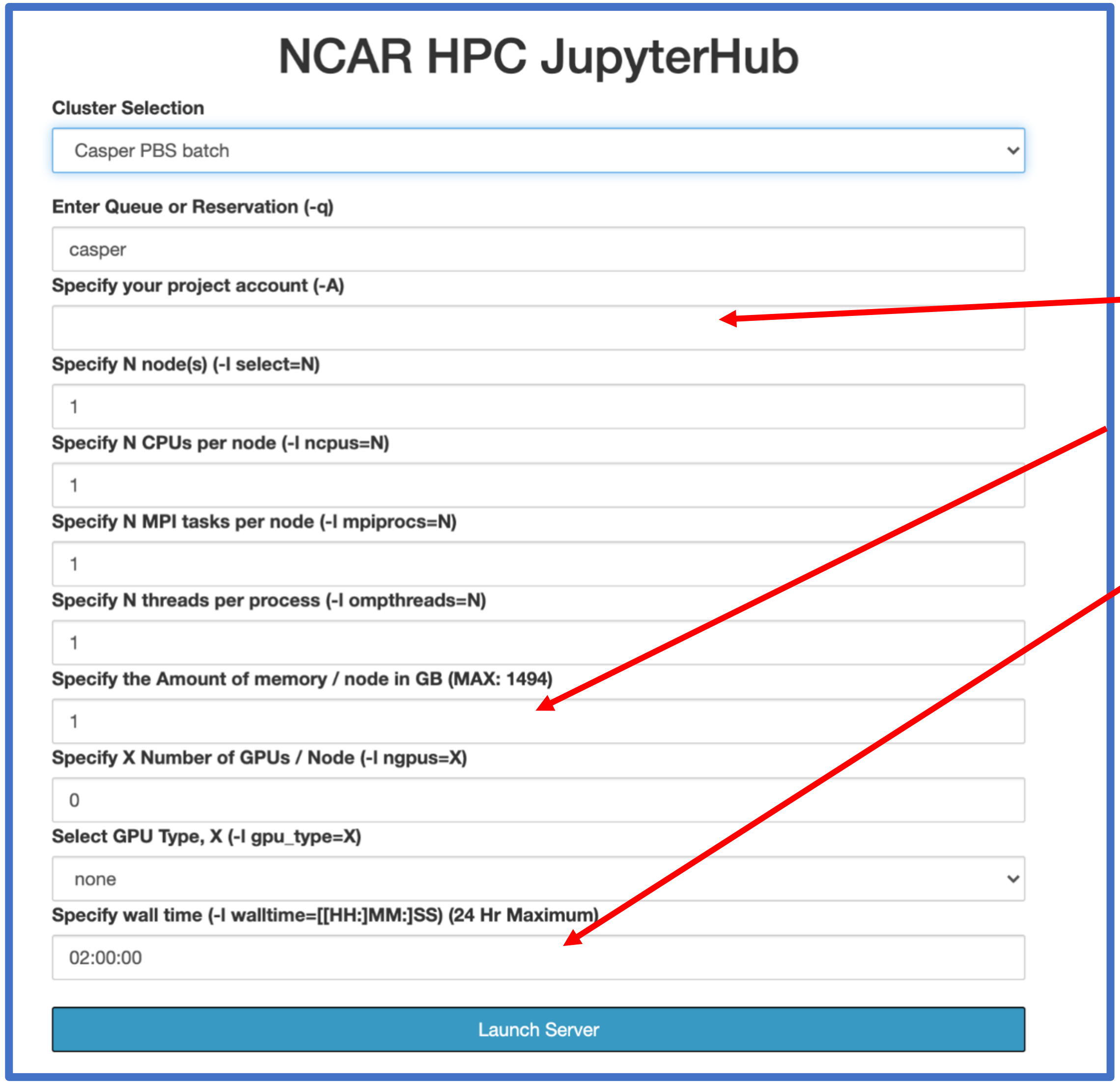
3. Login and start server



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





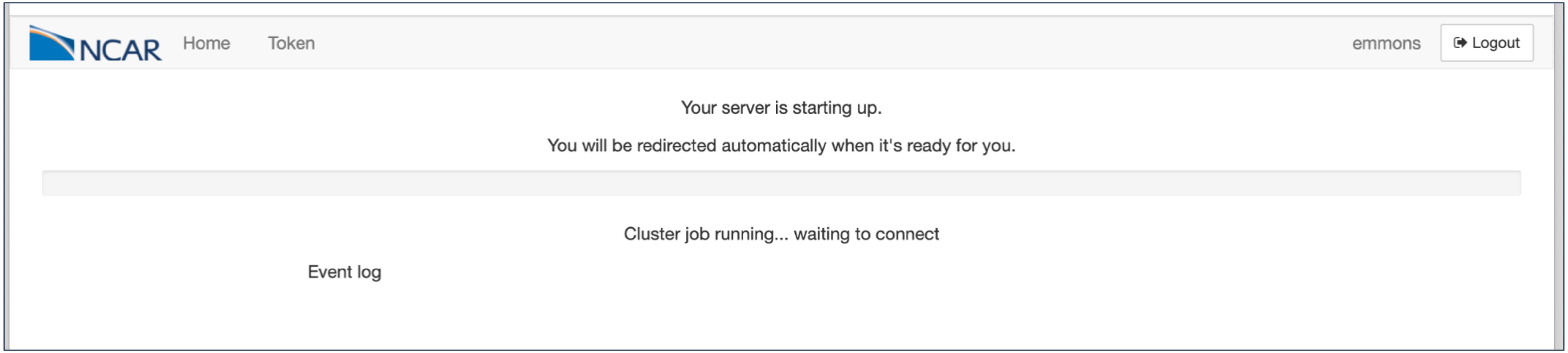
Enter your project number

You may need to increase memory, e.g. 15 GB

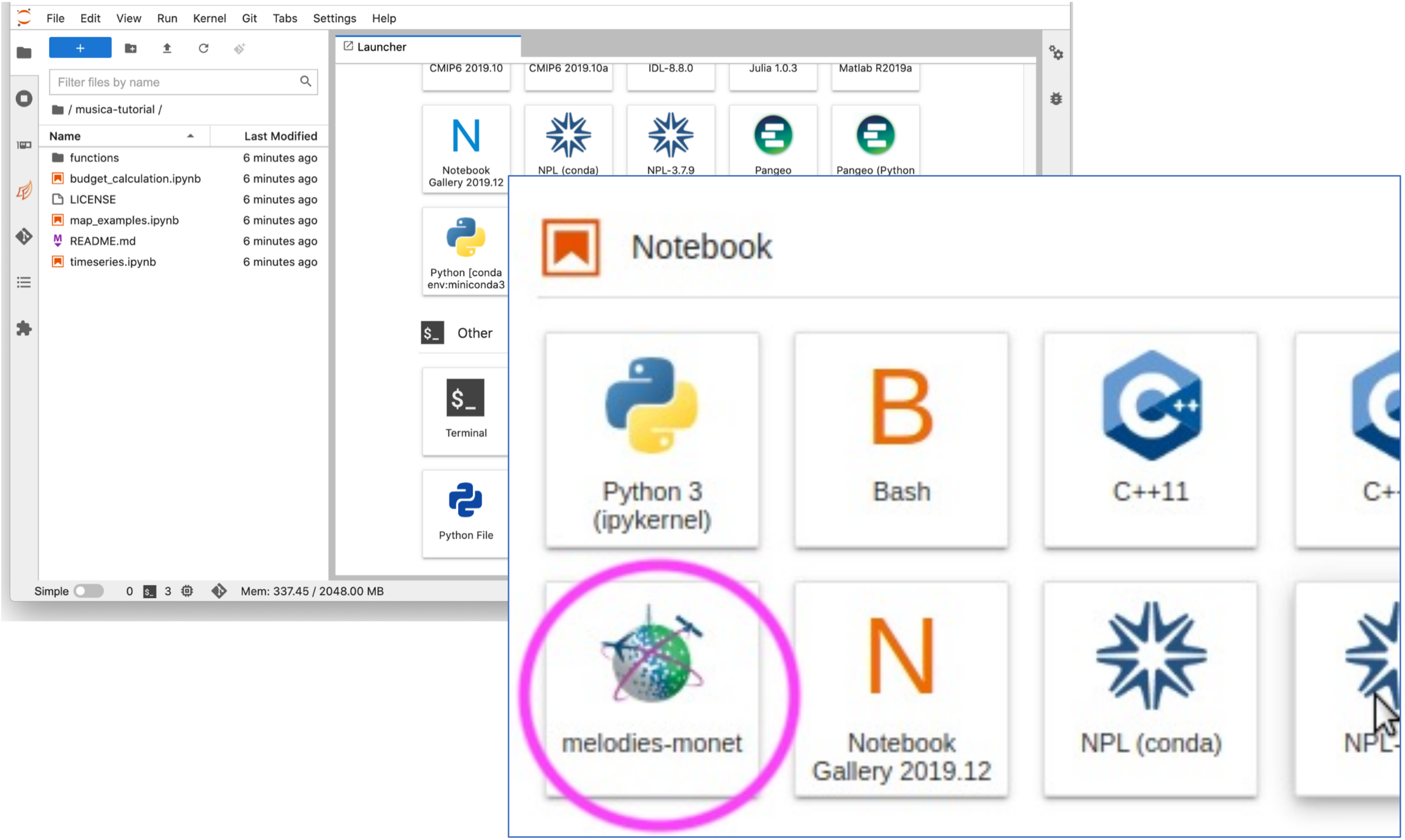
Increase wall-time only if needed

To reduce waiting time for Hub to start, use smallest memory and wall-time possible

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



In the Launcher window look for the ‘melodies-monet’ kernel.
Having this means you will also be able to select it from within your notebooks.



If **you do not have access to the ‘melodies-monet’ kernel**, you will need to create your own MELODIES MONET conda environment.

Follow the instructions at:

https://melodies-monet.readthedocs.io/en/latest/appendix/machine-specific-install.html#ncar-hpc-cheyenne-casper

You may wish to follow these instructions if you plan to develop new code and contribute it to the MELODIES-MONET repository.

If you have made your own melodies-monet conda environment on cheyenne/casper: you should see a kernel under the JupyterHub Notebooks “conda-melodies-monet” that you should use when running the MELODIES MONET notebooks.

If you prefer to install MELODIES MONET **on your own computer**, see:
https://melodies-monet.readthedocs.io/en/latest/tutorial/installation.html

Note: the instructions include ‘git clone’ commands using ssh, which assumes you have set up an ssh RSA key between cheyenne and your github account.
If you do not have that, you can use commands like:
> **git clone https://github.com/NOAA-CSL/MELODIES-MONET.git**
[instead of git clone git@github.com:NOAA-CSL/MELODIES-MONET.git]

Tutorial example notebooks:

- On cheyenne/casper: **/glade/p/acom/MUSICA/melodies_tutorial/notebooks/**
- https://drive.google.com/drive/folders/1-7NIQaUDlesGmGDU1P4VmlVIl4P68rdI?usp=sharing

Copy the *.ipynb and *.yaml files in either of these locations to somewhere in your home directory on casper (for example /glade/u/home/<username>/melodies_tutorial/; you can open a terminal from the JupyterHub launcher to do this).
Navigate within the JupyterHub file system display to that location and open a python notebook by double clicking (start with the mm_basics.ipynb).
Be sure to select the ‘melodies-monet’ kernel after you open the notebook.
Before trying to run the notebook, open the .yaml file that the notebook reads (e.g., mm_basics.yaml – it should be in the same directory as your notebook). Check that the paths for output, model results, observations are appropriate.
In the notebook, you may need to provide the full path to the yaml file.

When running tutorial notebooks:
Warnings related to “FutureWarning” after running “from melodies_monet import driver” can be ignored.

```
from melodies_monet import driver

/glade/u/home/cdswk/python/miniconda3/lib/python3.7/site-packages/dask/dataframe/utils.py:15: FutureWarning:
pandas.util.testing is deprecated. Use the functions in the public API at pandas.testing instead.
  import pandas.util.testing as tm
Please install s3fs if retrieving from the Amazon S3 Servers.  Otherwise continue with local data
Please install h5py to open files from the Amazon S3 servers.
Please install h5netcdf to open files from the Amazon S3 servers.
```

or if you don’t want to see warning messages:

```
# To ignore warning messages
import warnings
warnings.filterwarnings('ignore')

from melodies_monet import driver

Please install s3fs if retrieving from the Amazon S3 Servers.  Otherwise continue with local data
Please install h5py to open files from the Amazon S3 servers.
Please install h5netcdf to open files from the Amazon S3 servers.
```