While you wait

1. Connect to TAMU VPN and Login to Grace

```
ssh <username>@grace.tamu.edu
```

2. Go to your scratch directory

```
cd $SCRATCH
```

3. Clone the notebook repository from github

```
git clone https://github.com/abishekg7/python_geos.git
```

(OR)

Copy notebooks from Grace scratch

```
cp   -r    /scratch/training/python_geos/notebooks .
```

High Performance Research Computing
DIVISION OF RESEARCH

TEXAS A&M UNIVERSITY
Oceanography

Python Tools for Geosciences

Spring 2022 HPRC Short Course
Apr 1, 2022

Abishek Gopal
Assistant Research Scientist
iHESP, Texas A&M Oceanography
Texas A&M High Performance Research Computing

Expectations for this course

- Get an overview of some recent Python libraries designed to support geoscientific analysis
- Learn about the data structures in xarray, how to load and visualize netCDF files, and some basic operations
- Explore other geoscience packages built on top of xarray
- **Intended to be a starting point for switching your workflow to Python**

Helpful HPRC resources

- Grace quick start guide
  - https://hprc.tamu.edu/wiki/Grace:QuickStart
- Introduction to HPRC – Short course
  - https://hprc.tamu.edu/training/intro_hprc.html
- Submit tickets to help@hprc.tamu.edu

Upcoming relevant HPRC short courses

- Apr 8: Introduction to Fortran
  - **Instructor:** Abishek Gopal
  - **Time:** Friday, Apr 8, 10:00AM - 12:30PM
- Apr 8: Introduction to Perl
  - **Instructor:** Keith Jackson
  - **Time:** Friday, Apr 8, 1:30PM - 4:00PM
- Apr 8: Introduction to Code Parallelization using MPI and OpenMP
  - **Instructor:** Marinus Pennings
  - Opens Friday, Apr 8 on Google Classroom

https://hprc.tamu.edu/training/index.html

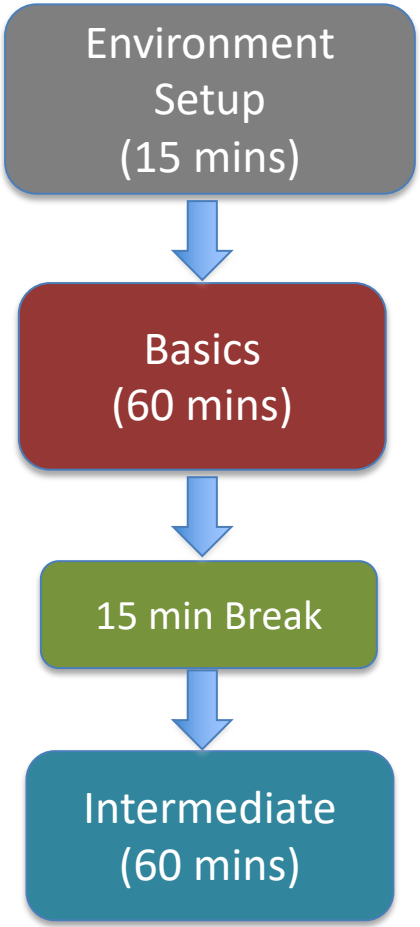
Acknowledgements

- Course materials adapted from detailed xarray, xgcm and Siphon tutorial notebooks
  - https://github.com/xarray-contrib/xarray-tutorial
  - https://gallery.pangeo.io/repos/xgcm/xgcm-examples/
  - https://unidata.github.io/siphon/latest/examples/index.html
- The HPRC team supporting the short course operations

- Sanjiv R., Steve Y., Fred C., Dapeng Li (iHESP)

- Kristen Thyng (previously: TAMU, now: Axiom Data Science)

Course outline



- Intro to the Pangeo stack
- xarray data structures
- Reading and writing netCDF files

- Plotting with matplotlib and cartopy
- Spatial operations in xgcm
- Data access using Siphon

Launching a JupyterLab notebook from Grace portal

High Performance Research Computing
DIVISION OF RESEARCH

1. Go to https://portal.hprc.tamu.edu/

High Performance Research Computing
A Resource for Research and Discovery
TEXAS A&M UNIVERSITY

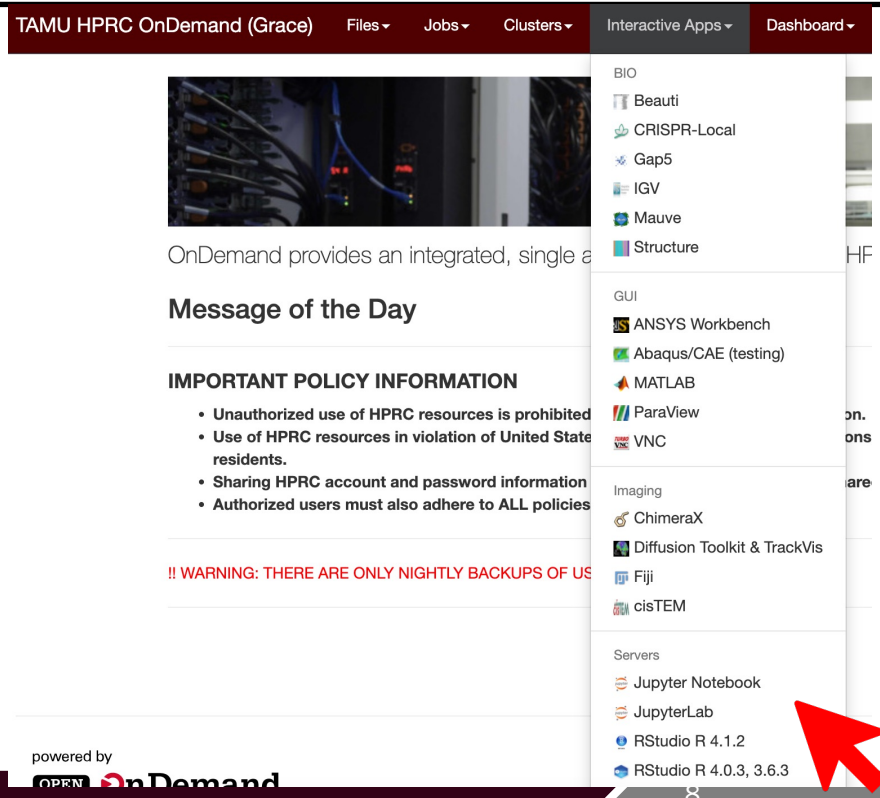
TAMU HPRC OnDemand Homepage

Terra OnDemand Portal

Grace OnDemand Portal

OnDemand Portal User Guide

2. Interactive Apps -> JupyterLab



JupyterLab

This app will launch a JupyterLab server on the Grace cluster.

Module

Anaconda3/5.3.0

Anaconda/3-x.x.x.x and Anaconda3 use Python3

Optional Environment to be activated

/scratch/training/python_geos/conda/envs/training

Enter the name of the environment to be activated. (Optional)

Number of hours

3

Number of cores:

4

Specify the number of cores [1–48] allocated on a node from the Grace cluster.

Total memory (GB)

30

Requested total memory (2 - 360GB)

Launch

* The JupyterLab session data for this session can be accessed under the data root

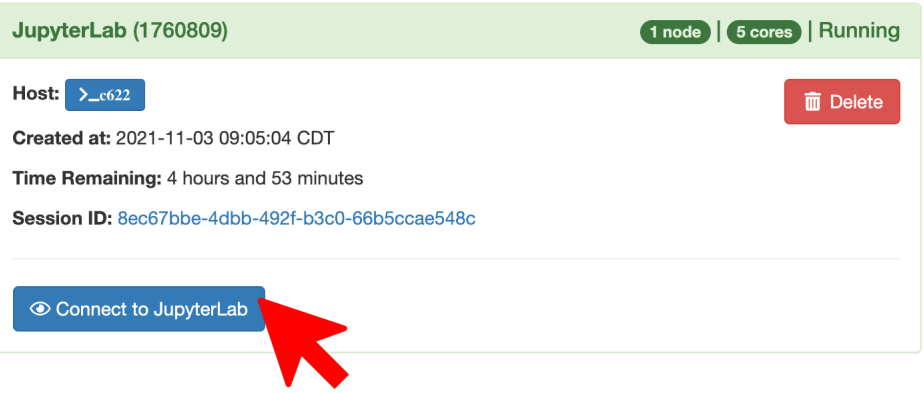
Enter environment path

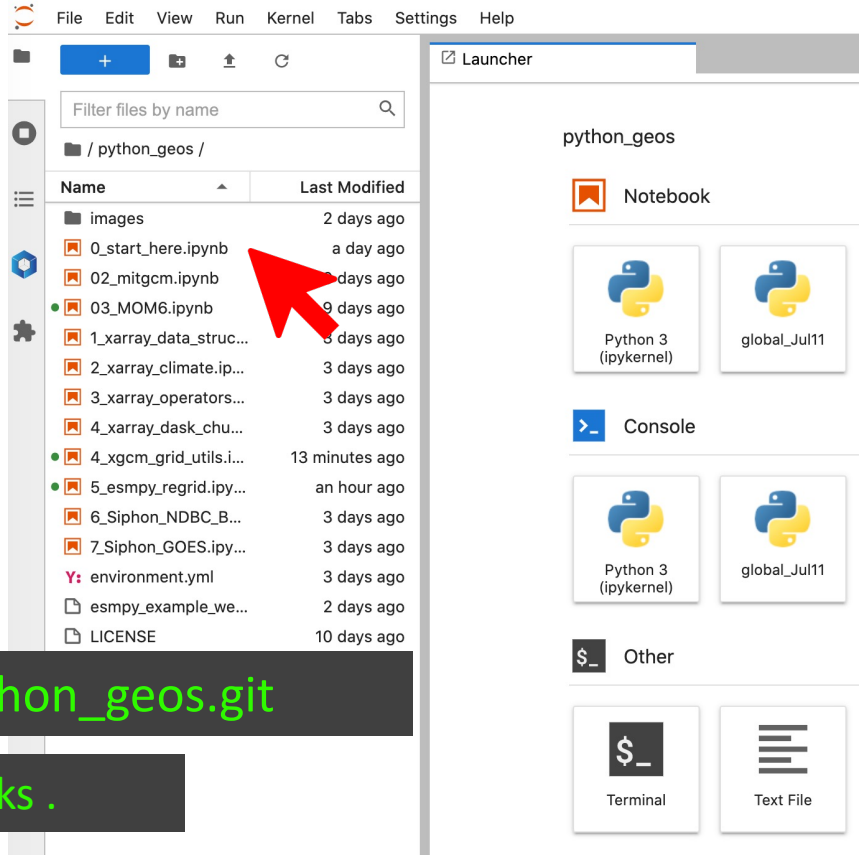
/scratch/training/python_geos
/conda/envs/training

Request 3 cores/ 30 GB
for 3 hours

Hit Launch

Connect to JupyterLab session



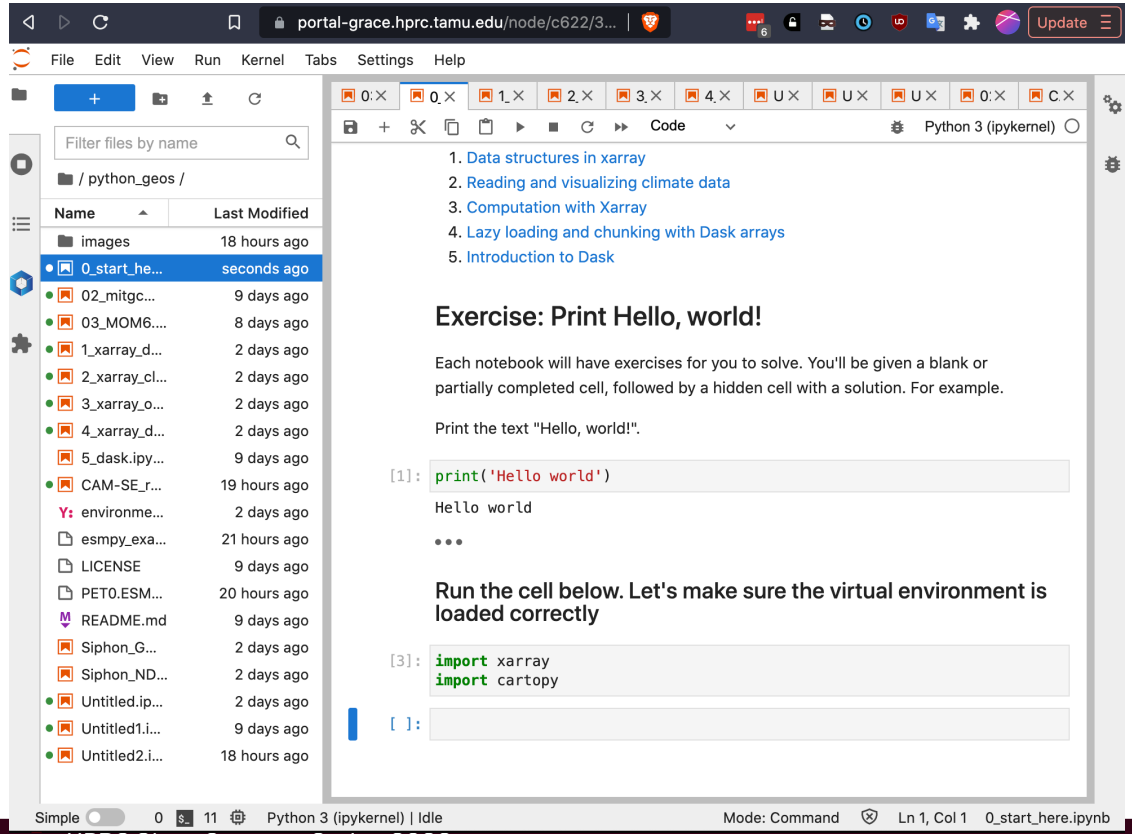



```
cd $SCRATCH
```

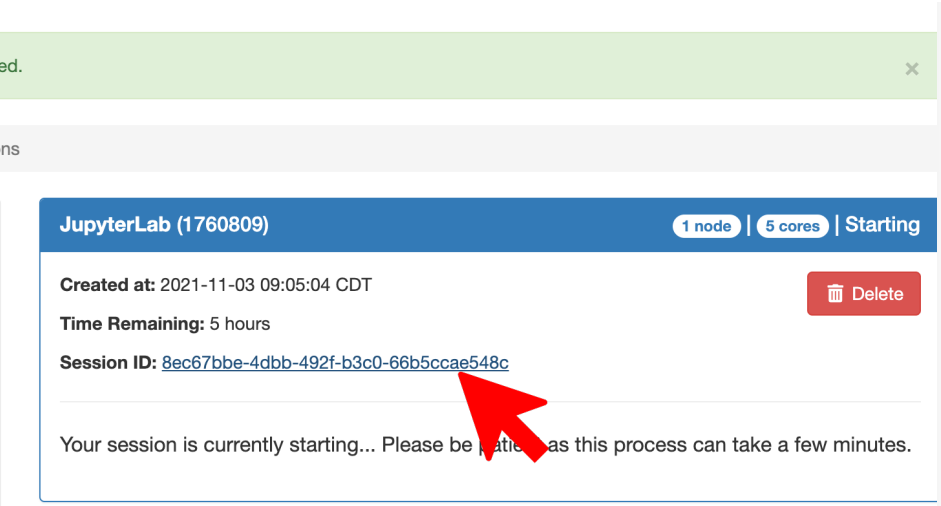
```
git clone https://github.com/abishekg7/python_geos.git
```

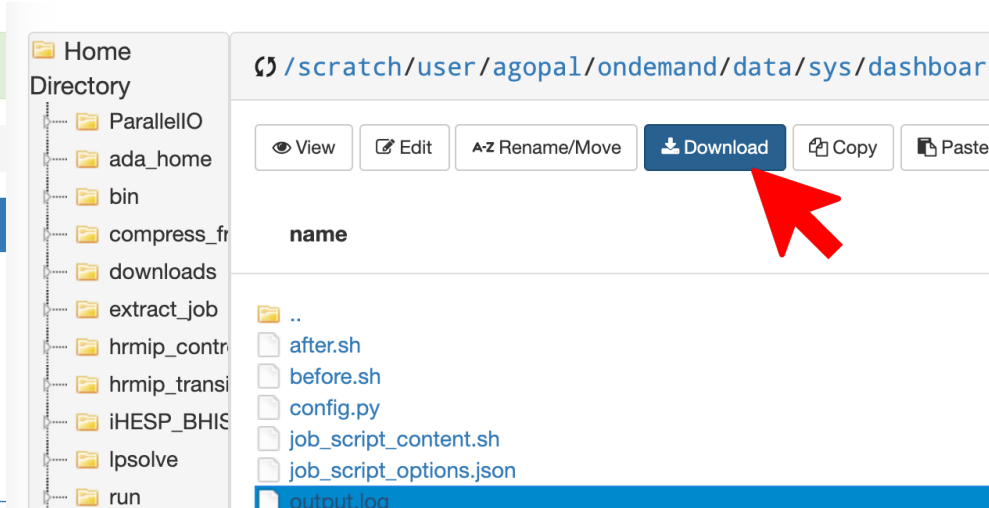
```
cp  -r  /scratch/training/python_geos/notebooks .
```

Check if the virtualenv works correctly



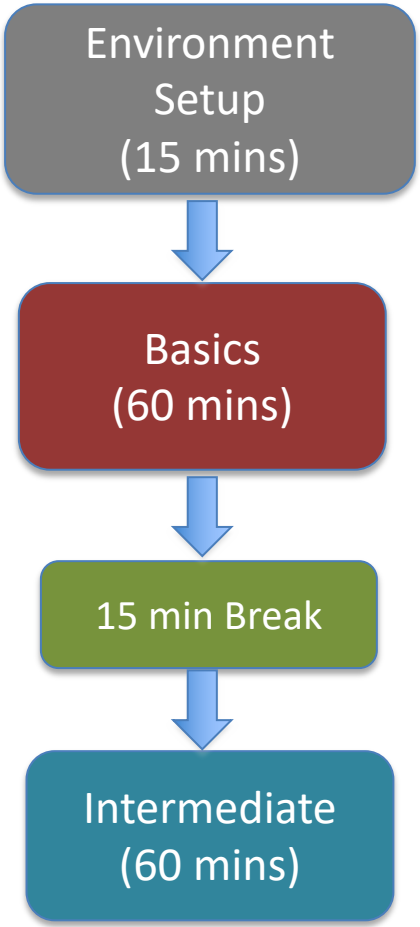
In case of session not starting or virtualenv issues





Email output.log to help@hprc.tamu.edu

Course outline



- Intro to the Pangeo stack
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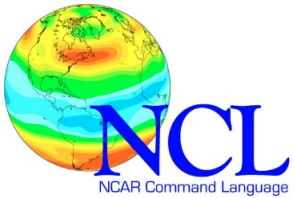
Current/last generation of post-processing tools



NOAA/ PMEL
FERRET

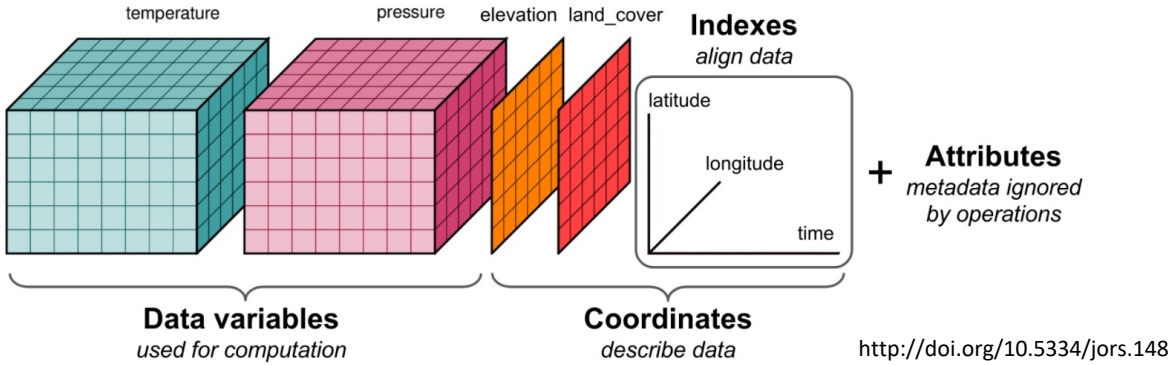
Max-Planck-Institut für Meteorologie CDO

- Mature tools/languages for working with moderate resolution datasets
- Often optimized to do specific tasks really well/fast.
- Not designed with high-resolution datasets in mind.

Python geo-scientific software stack

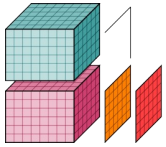
Credit: Ryan Abernathey. Inspired by Jake VanderPlas PyCon 2019

"pandas for N-dimensional arrays"



http://doi.org/10.5334/jors.148

- Builds on NumPy by applying metadata such as dimensions, coordinates, data variables and attributes to raw NumPy arrays.
- Inherits Pandas functionality
- xarray.Dataset is an in-memory representation of the netCDF file format
- xarray works seamlessly with the dask library to enable parallel computations more easily



xarray

Apply operations over named dimensions

```
x.sum('time')
```

Select values by label or logical conditions, instead of integer location

```
x.loc['2014-01-01']
x.sel(time='2014-01-01')
```

Easily use the split-apply-combine paradigm with groupby

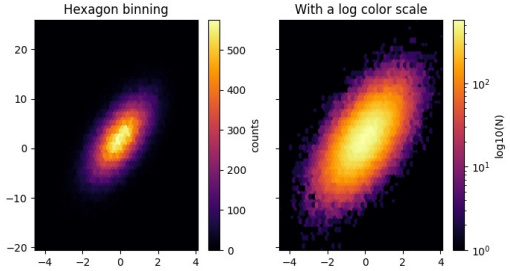
```
x.groupby('season').mean()
```

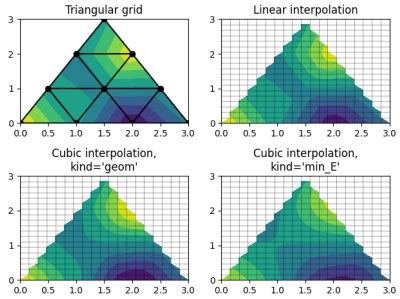
Keep track of arbitrary metadata in the form of a Python dictionary

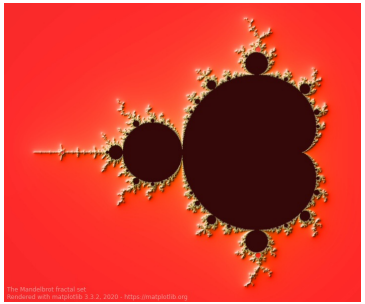
```
x.attrs
```

matplotlib

A comprehensive library for creating static, animated, and interactive visualizations in Python.



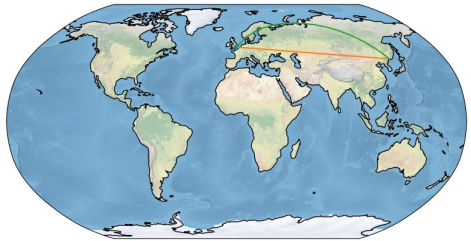


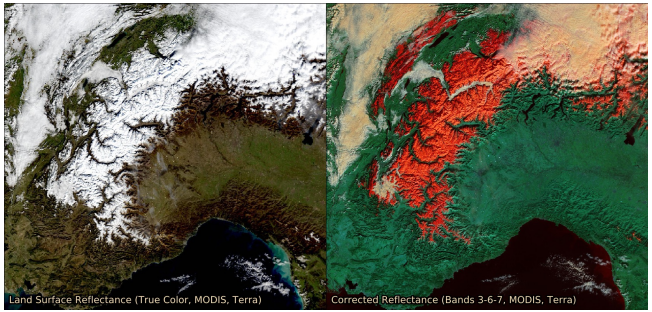


https://matplotlib.org/gallery/

Cartopy

Cartopy adds understanding of map projections to matplotlib plots



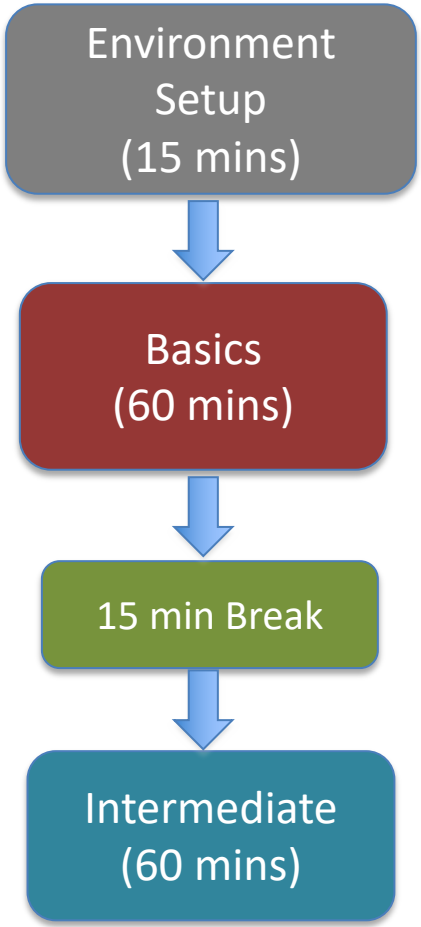


https://scitools.org.uk/cartopy/docs/latest/gallery/index.html

Short break!
(15 minutes)

We will resume at 2:45 Central

Course outline



- Intro to the Pangeo stack
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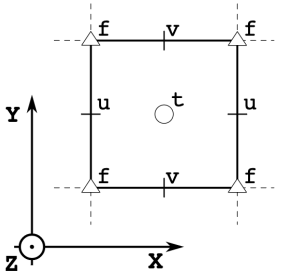
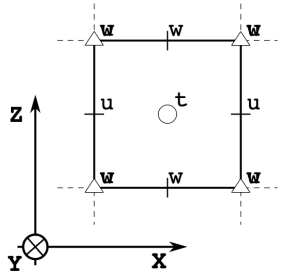
GCM

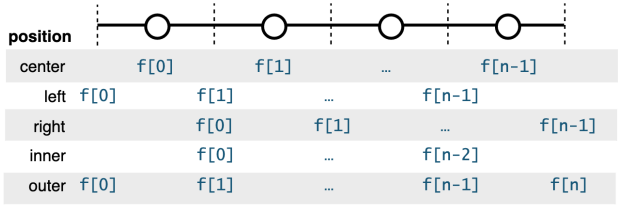
- xarray doesn't implicitly understand GCM grids
- xgcm wraps xarray to add an understanding of grid topology
- Implements spatial derivative operators
- Understands only C-grids for now, but other works are in progress
- Grid-aware vertical interpolation



C-grid — horizontal view



C-grid — vertical view

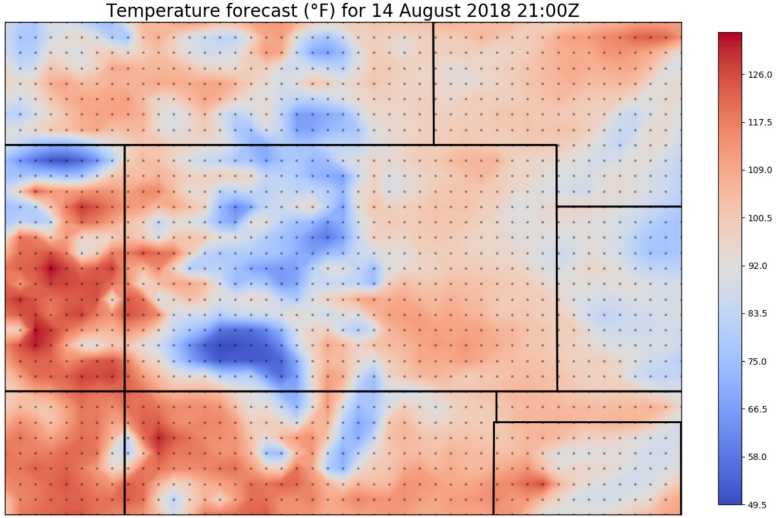


The different possible positions of a variable `f` along an axis.

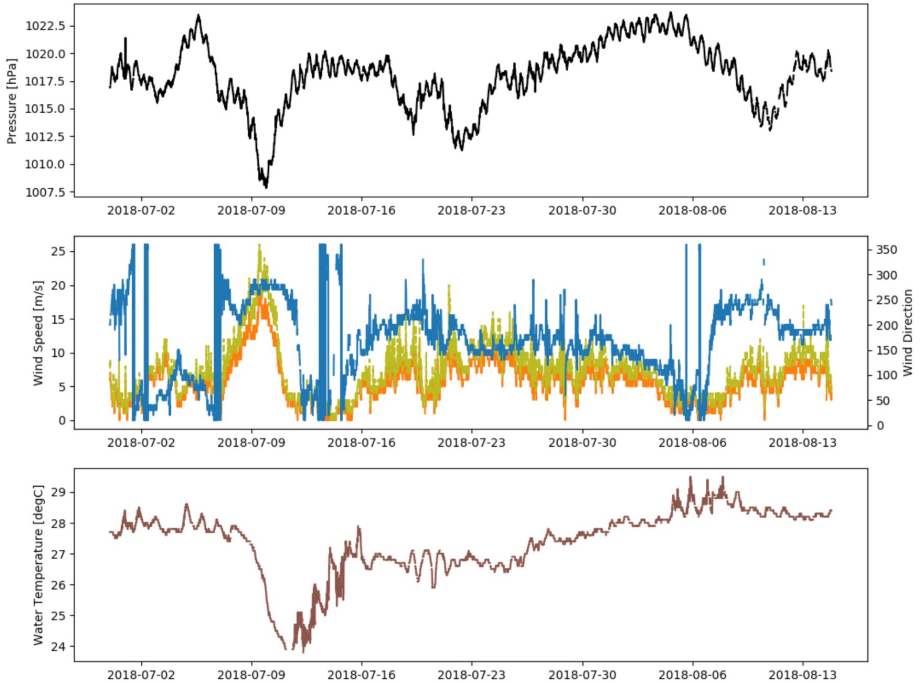
https://xgcm.readthedocs.io/en/latest/grids.html

A collection of Python utilities for downloading data from remote data services

Siphon



https://matplotlib.org/gallery/



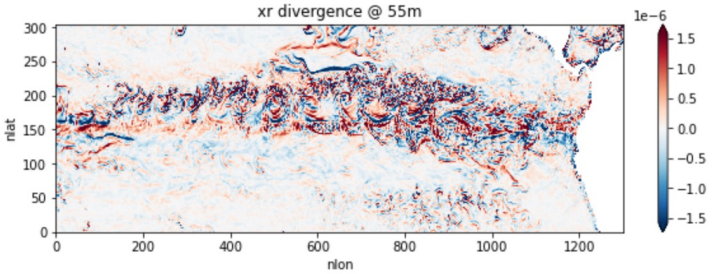
https://scitools.org.uk/cartopy/docs/latest/gallery/index.html

Some great Python modules to go along with xarray and dask!

pop-tools

Tools to support analysis of POP2-CESM model solutions with xarray

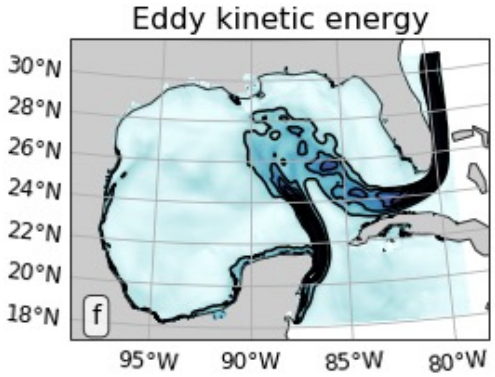
- Wraps xgcm to provide support for POP2 grids.
- Inherits spatial derivative operators from xgcm
- Support for POP2 region masks

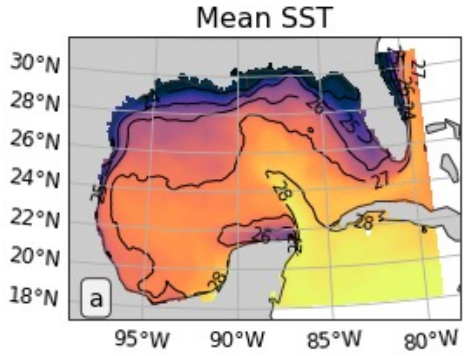


https://pop-tools.readthedocs.io/en/latest/

xroms

- Wraps xgcm to provide ROMS-specific grid manipulations and functions of interest to oceanographers.
- Developed by Kristen Thyng, Rob Hetland, et al. at TAMU
- Wraps **cf-xarray** to generalize coordinate and dimension calling.
- Wraps **xcmocean** to automatically choose colormaps for plotting!

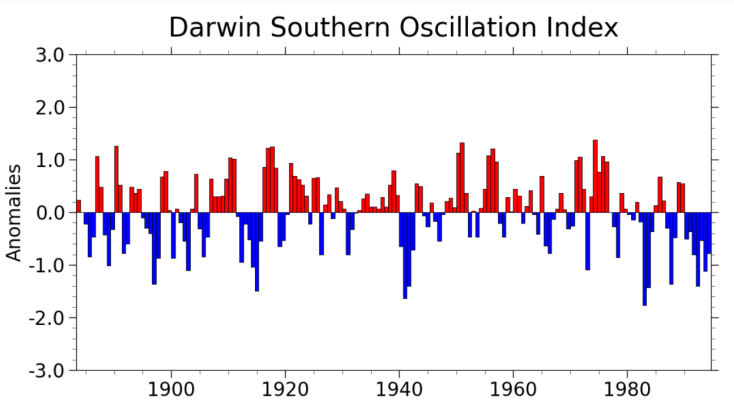


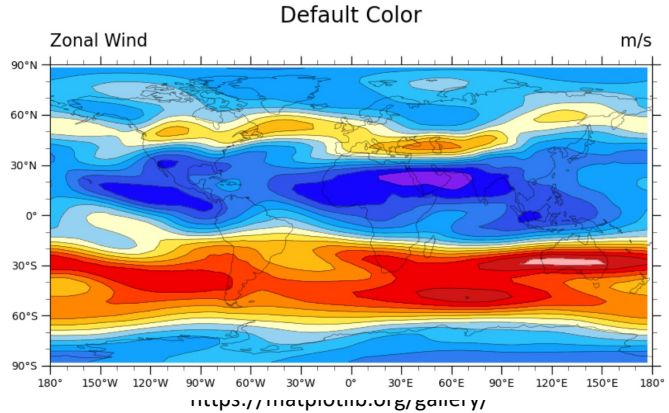


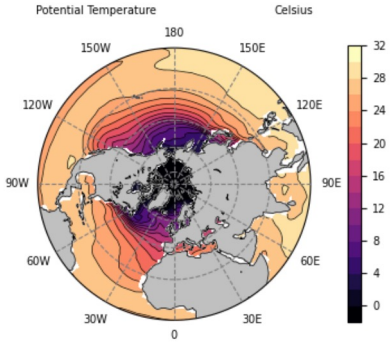
https://github.com/kthyng/xroms

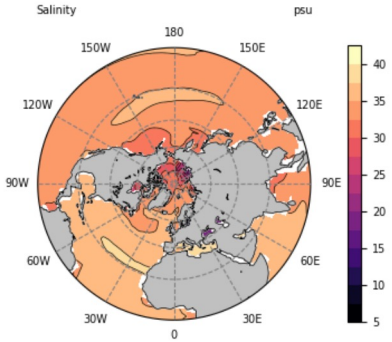
GeoCAT

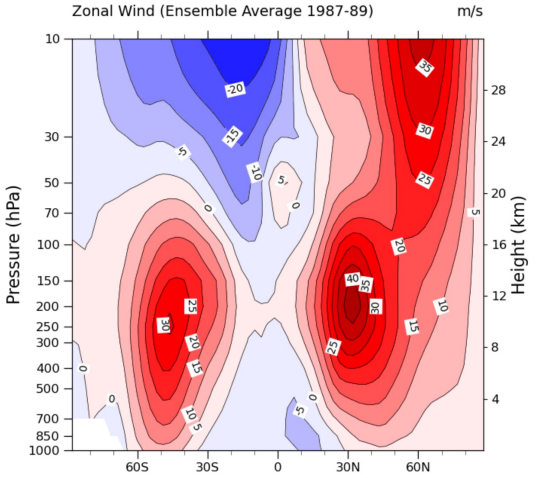
A collection of Python utilities related to NCL





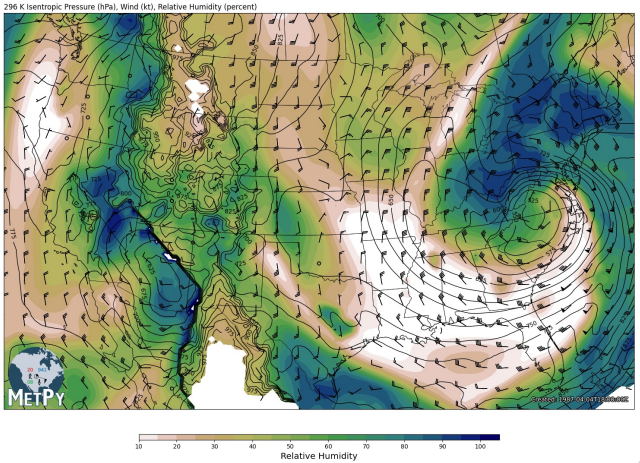


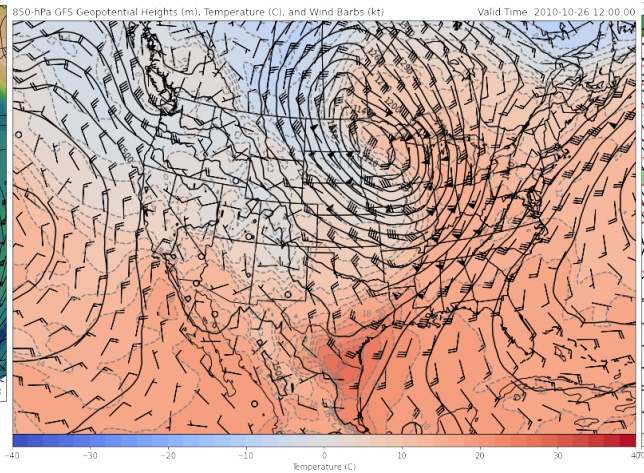


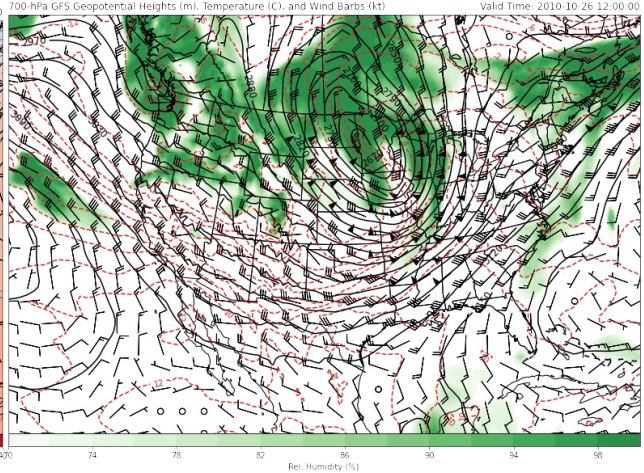


https://geocat-examples.readthedocs.io/en/latest/gallery/index.html

A collection of Python tools for reading, visualizing, and performing calculations with weather data.







https://unidata.github.io/python-training/gallery/gallery-home/

Key Takeaways

- The Pangeo framework rethinks how we analyze large datasets
  - Resusable software design can help avoid re-writing analysis scripts that has already been developed by community
  - In its developmental stages, and will take a few more years to reach the depth/breadth of existing geoscience tools
  - For newer analysis tools development, consider using Pangeo

- NCO, CDO, Ferret, etc are still extremely handy for specific tasks

Additional Python resources

- Previously offered HPRC short courses
  - Introduction to Python
    - https://hprc.tamu.edu/training/intro_python.html
  - Introduction to Scientific Python
    - https://hprc.tamu.edu/training/intro_scientific_python.html
  - Introduction to Python for MATLAB users
    - https://hprc.tamu.edu/training/python_matlab.html

- NumPy for MATLAB users (Quick reference)
  - http://mathesaurus.sourceforge.net/matlab-numpy.html

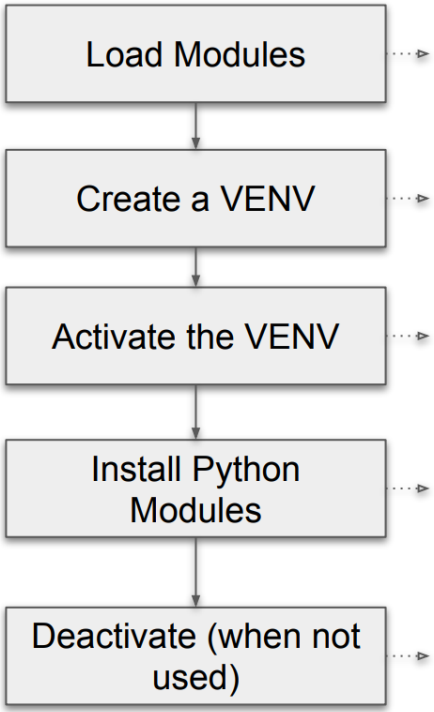
Additional resources

- Official Documentation
  - xarray docs
  - xgcm docs

- Ask for help:
  - Use the python-xarray on StackOverflow
  - GitHub Issues for bug reports and feature requests
  - Pangeo forums http://discourse.pangeo.io/

Questions?

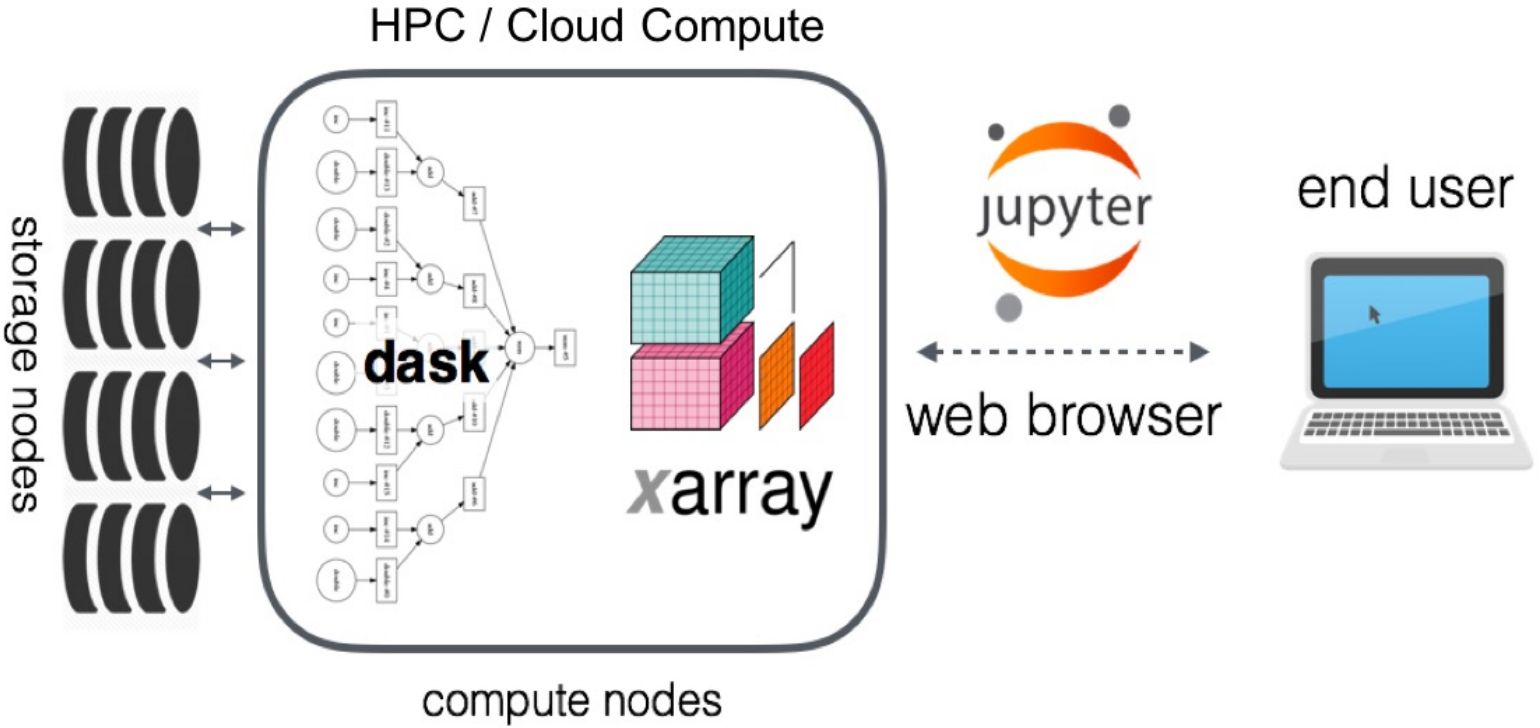
Conda virtual environment




```
cd $SCRATCH
# Load Anaconda
ml Anaconda3/2020.07

# Create the virtual environment
conda create python=3.7 -n training -c conda-forge

# Activate the virtual environment
source activate training

# Install packages into the virtual environment
conda install -c conda-forge cartopy matplotlib xarray
conda install -c conda-forge xgcm dask esmpy

# Deactivate the environment
source deactivate
```

Pangeo

https://pangeo.io/architecture.html



BUILD YOUR OWN PANGEO

Storage Formats	HDF	OPeNDAP	Cloud Optimized COG/Zarr/Parquet/etc.
ND-Arrays	NumPy	DASK	More coming…
Data Models	xarray	Iris	pandas
Processing Mode	jupyter Interactive	Batch 	Serverless
Compute Platform	HPC 	Cloud  Google Cloud Platform	Local

https://www.ecmwf.int/sites/default/files/elibrary/2018/18737-why-pangeo-what-it-and-why-we-need-it.pdf

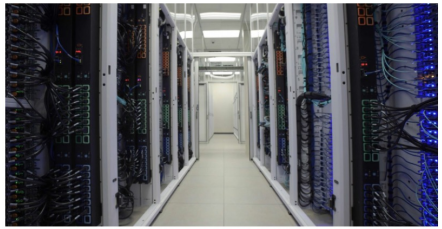
Launching a JupyterLab notebook from Grace portal

High Performance Research Computing
DIVISION OF RESEARCH

1. Go to https://portal.hprc.tamu.edu/

High Performance Research Computing
A Resource for Research and Discovery
TEXAS A&M UNIVERSITY

TAMU HPRC OnDemand Homepage

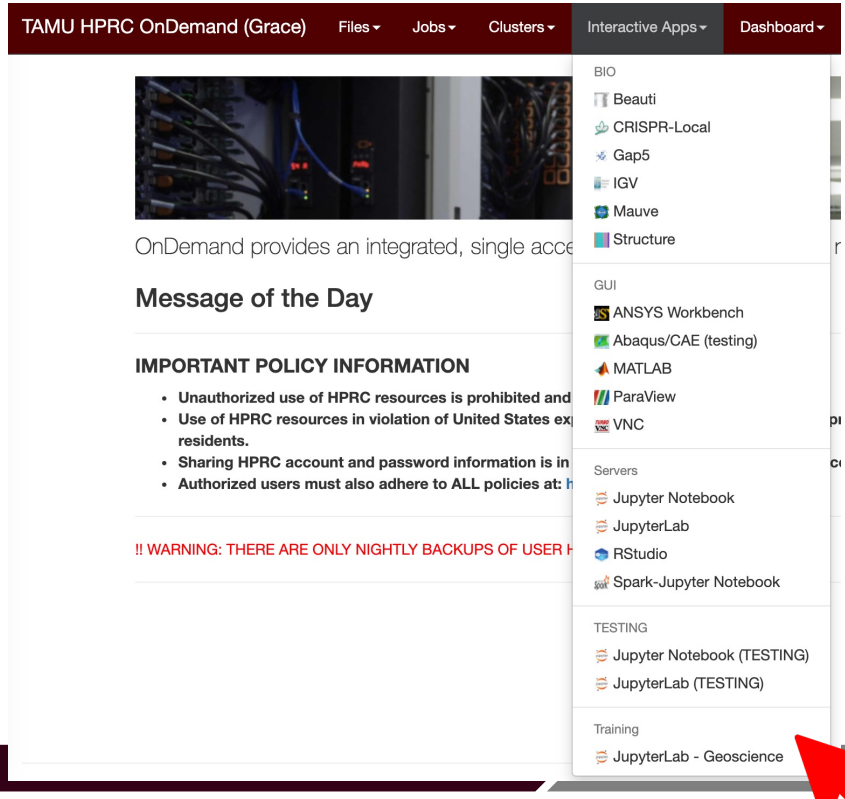


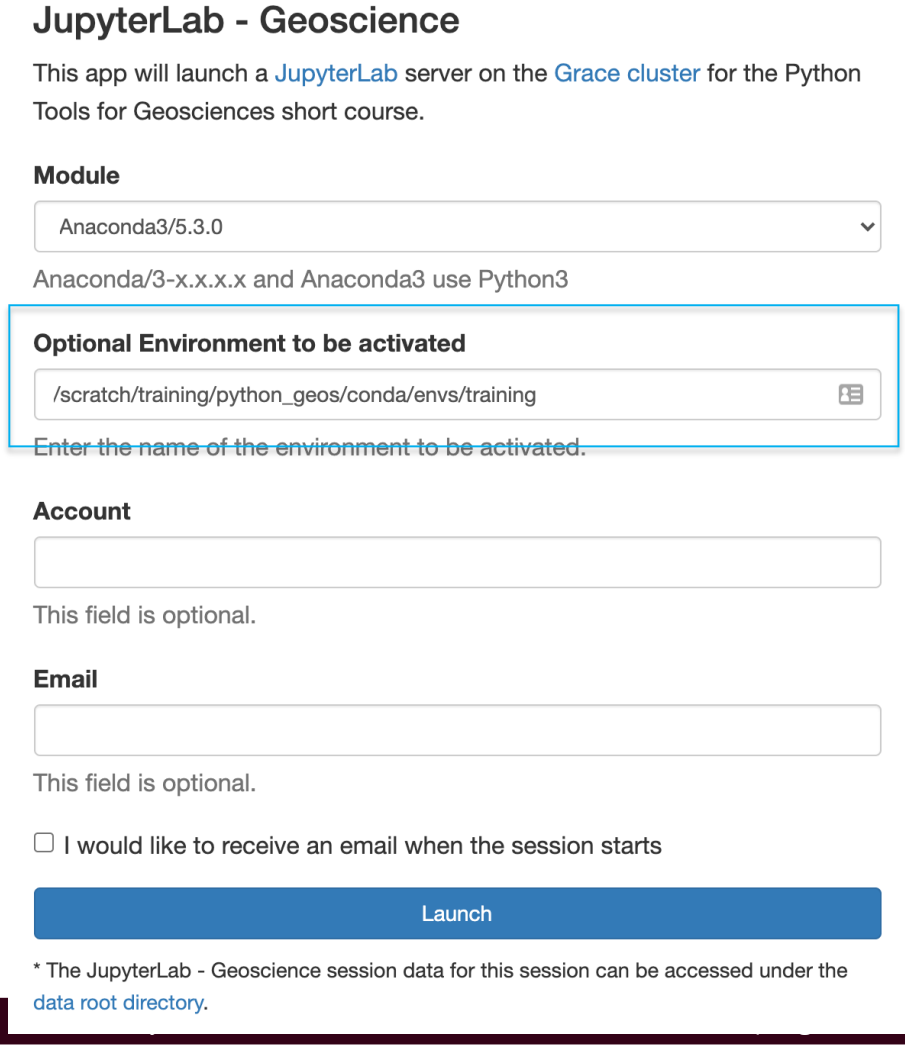
Terra OnDemand Portal

Grace OnDemand Portal

OnDemand Portal User Guide

2. Interactive Apps -> JupyterLab Geoscience





Check environment path

/scratch/training/python_geos /conda/envs/training

Hit Launch