High Performance
Research Computing
DIVISION OF RESEARCH

TEXAS A&M UNIVERSITY
Oceanography

Post-processing CESM model output using Python-based utilities

Spring 2020 HPRC Short Course
April 10, 2020

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Helpful HPRC resources

- Ada quick start guide
  - https://hprc.tamu.edu/wiki/Ada:QuickStart
- Introduction to the Ada and Terra clusters – Short course (Spring 2020)
  - https://hprc.tamu.edu/files/training/2020/Spring/Intro_to_HPRC_clusters_2020_spring.pdf
- Submit tickets to help@hprc.tamu.edu

Upcoming HPRC short courses

- **Introduction to Entos - QM Simulation Software for PCs, HPC, and the Cloud**
  - **Instructor:** Thomas Miller (Professor at Caltech and Entos co-founder) and Daniel Smith (Entos)
  - **Time:** Friday, April 10, 1:30PM-4:00PM
- **Searching for the Cure – COVID-19 Classical Molecular Dynamics with NAMD**
  - **Instructor:** Dr. Lisa M. Perez
  - **Time:** Friday, April 17, 10:00AM-12:30PM
- **Searching for the Cure – COVID-19 Drug Docking with AutoDock and Schrödinger**
  - **Instructor:** Dr. Lisa M. Perez
  - **Time:** Friday, April 17, 1:30PM-4:00PM

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

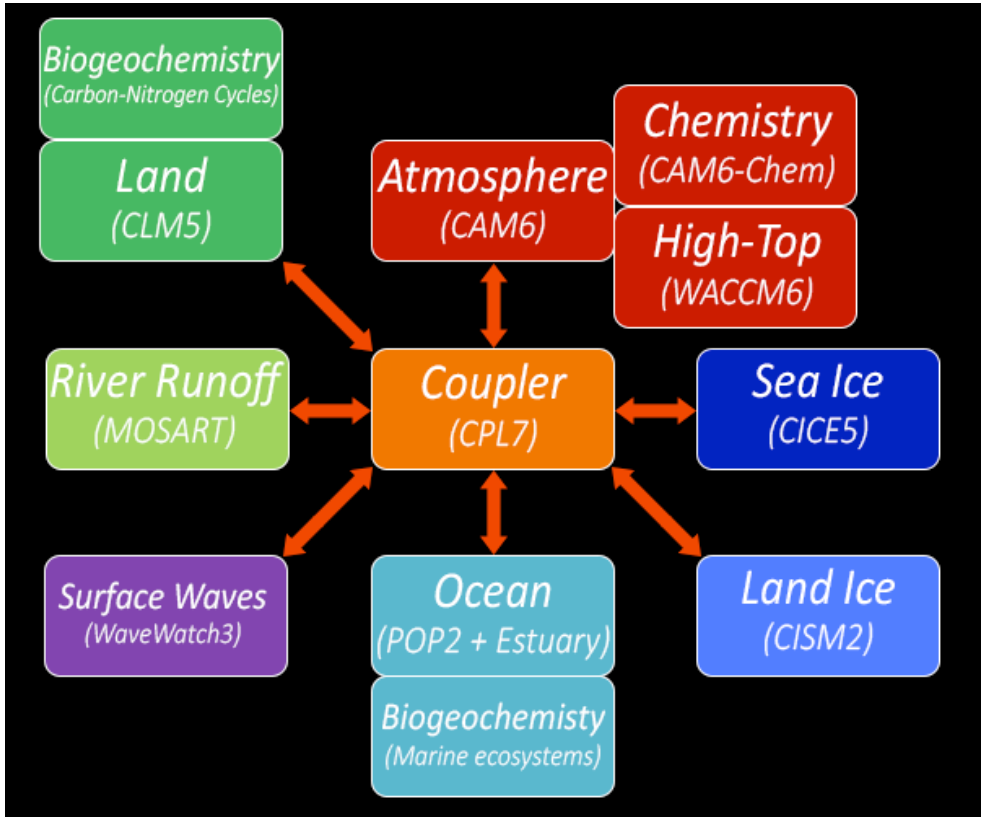
Course structure

- Structure of CESM model output and netCDF format
- Installing and configuring the CESM_postprocessing package
- Generating time-averages and climatology files
- Short break (15 minutes)
- Generating diagnostics of CESM model runs
- Pangeo for geosciences
- Loading and visualizing datasets using xarray and cartopy
- Speeding up computations using dask

Expectations for this course

- Learn about performance benefits of parallel python tools in generating climatology files
- Learn about the available diagnostic plots sets
- Get some hands-on experience with the CESM diagnostics tool
- Learn about the future trends in using Python for geosciences

The Community Earth System Model (CESM)

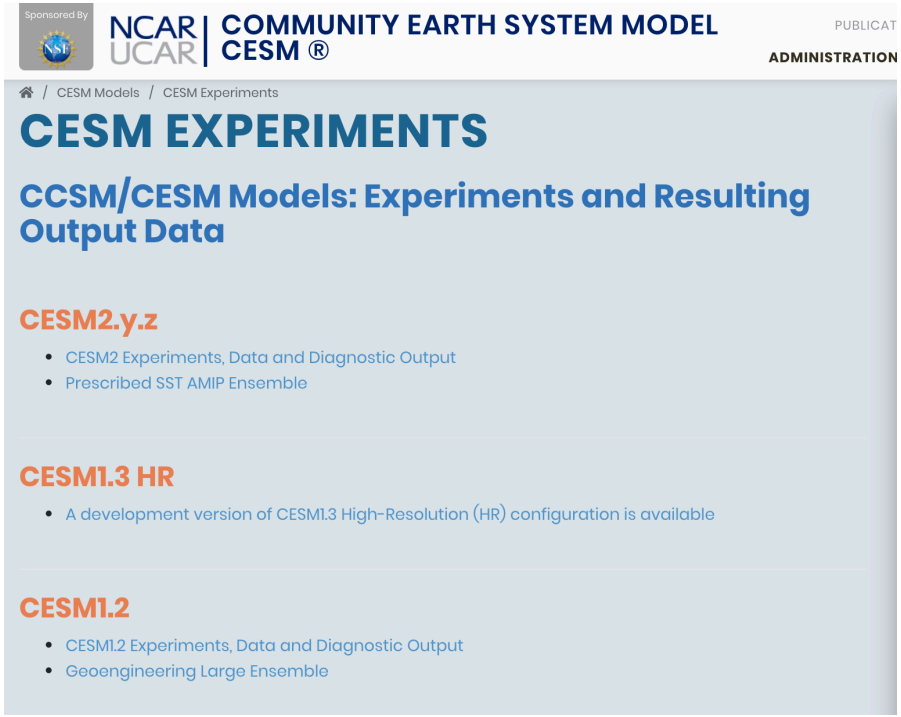


https://nar.ucar.edu/2017/cgd/development-cesm2

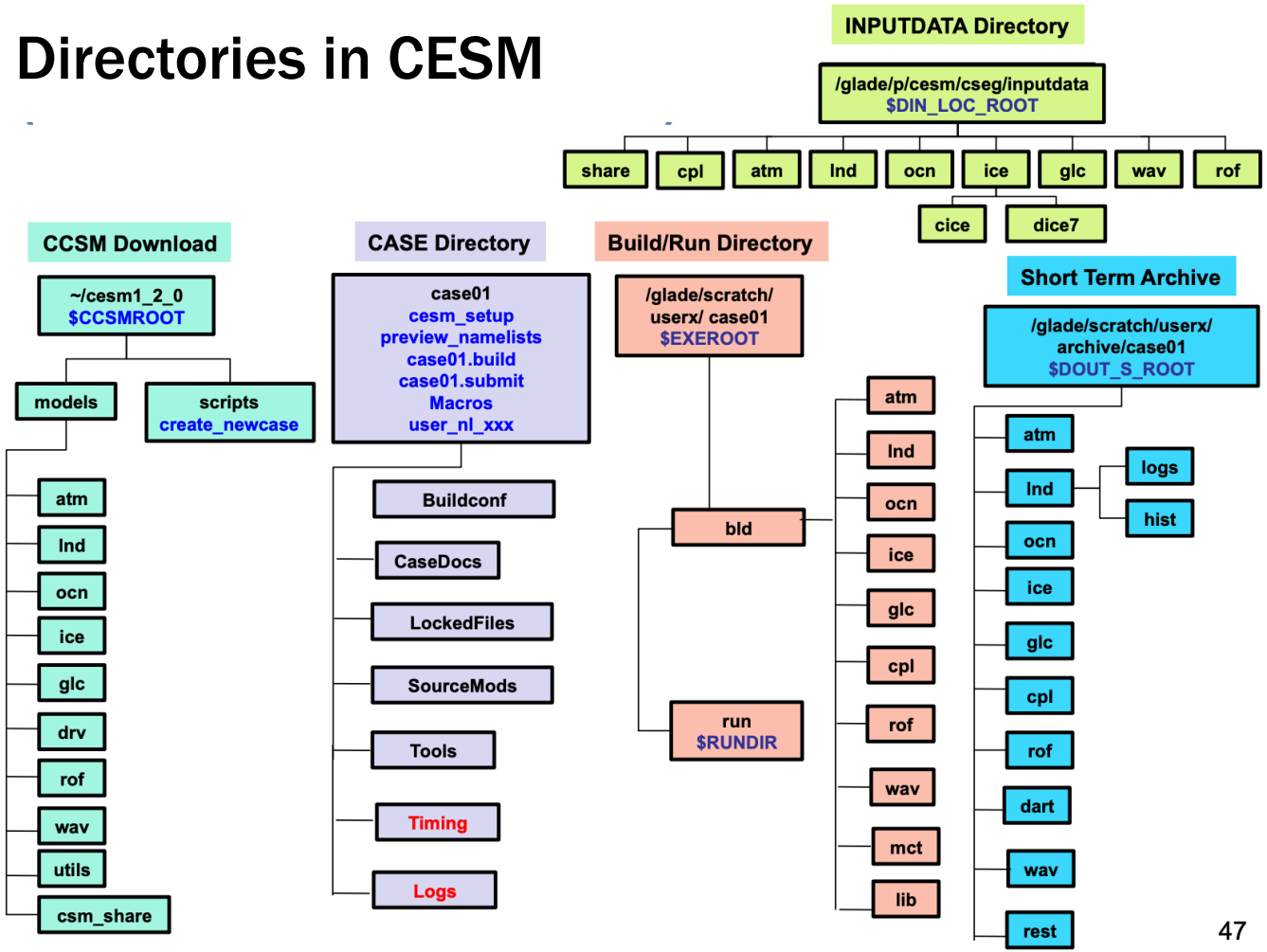
Publicly available CESM model output

- http://www.cesm.ucar.edu/experiments/
- https://www.earthsystemgrid.org/

Sample datasets for the tutorial available on Ada at /scratch/training/CESM_post/datasets



Directories in CESM



http://www.cesm.ucar.edu/models/cesm1.2/cesm/cesm1_tutorial_130619_full.pdf

47

History vs Timeseries format

- History files contain a set of variables output at a given time slice in a single file.
- Timeseries files contain single variable data for all times
- CESM writes model output in short-term archive as history files
- Variables with larger dimensions (Ex: TEMP) are usually output as a lower frequency history files, than smaller variables (Ex: SST).
- Timeseries files are usually shared publicly.
- How to transpose history files to timeseries files?

CESM Case naming convention

<compset char>.<code base>.<compset sname>.<resolution sname>
[.opt_desc_string].<nnn>[opt_char]

<compset char>	= 1 character, first letter of compset
<code base>	= code base, “e20” for cesm2.0, “e10” for cesm1.0, ”c40” for ccsm4.0, and “c35” for ccsm3.5.
<compset sname>	= compset shortname
<resolution sname>	= resolution shortname
<.opt_desc_string>	= optional descriptive string, to be kept short if possible
<nnn>	= 3 digit number
[opt_char]	= optional single lower-cased letter; allowed to distinguish a group of cases that are very closely related

Examples: b.e21.B1850.f09_g16.CMIP6-piControl.001
f.e11.FAMIPCN.f09_f09.rcp85_ersstv5.005

One note about compsets: The first letter of the casename is indicative of the type of run it is: A coupled run (A “B” case), an atmosphere/land run (“F”), a land run (“I”), or an ocean/ice run (“G”). Other letters (A,Q,S,T,X) denoting less common configurations are also used.

Adam Phillips, NCAR

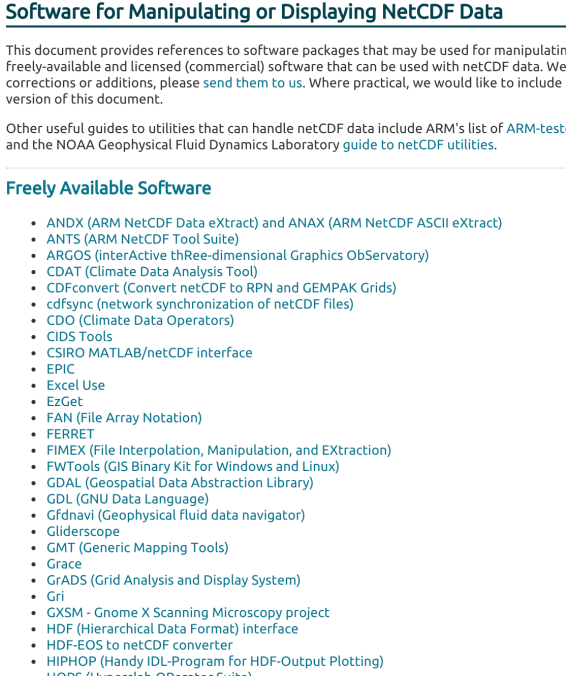
NetCDF format

```
netcdf pres_temp_4D {
  dimensions:
                  level = 2 ;
                  latitude = 6 ;
                  longitude = 12 ;
                  time = UNLIMITED ;
  variables:
                  float latitude(latitude);
                          latitude:units = "degrees_north" ;
                  float longitude(longitude) ;
                          longitude:units = "degrees_east" ;
                  float pressure(time, level, latitude, longitude) ;
                          pressure:units = "hPa" ;
                  float temperature(time, level, latitude, longitude) ;
                                          temperature:units = "celsius" ;
  data:
                  latitude = 25, 30, 35, 40, 45, 50 ;
                  longitude = -125, -120, … ;
                  pressure = 900, 901, 902, … ;
                  temperature = 9, 10, 11, …;
}
```

https://www.archer.ac.uk/training/course-material/2015/01/data_mgmt_epcc/netcdf.pdf

Tools to process and visualize NetCDF files

- NetCDF Operators (NCO)
- Climate Data Operators (CDO)
- NCAR Command Language (NCL)
- MATLAB
- Interactive Data Language (IDL)
- Panoply (from NASA GISS)
- PyNGL and PyNIO



Software for Manipulating or Displaying NetCDF Data

This document provides references to software packages that may be used for manipulatin
freely-available and licensed (commercial) software that can be used with netCDF data. We
corrections or additions, please send them to us. Where practical, we would like to include
version of this document.

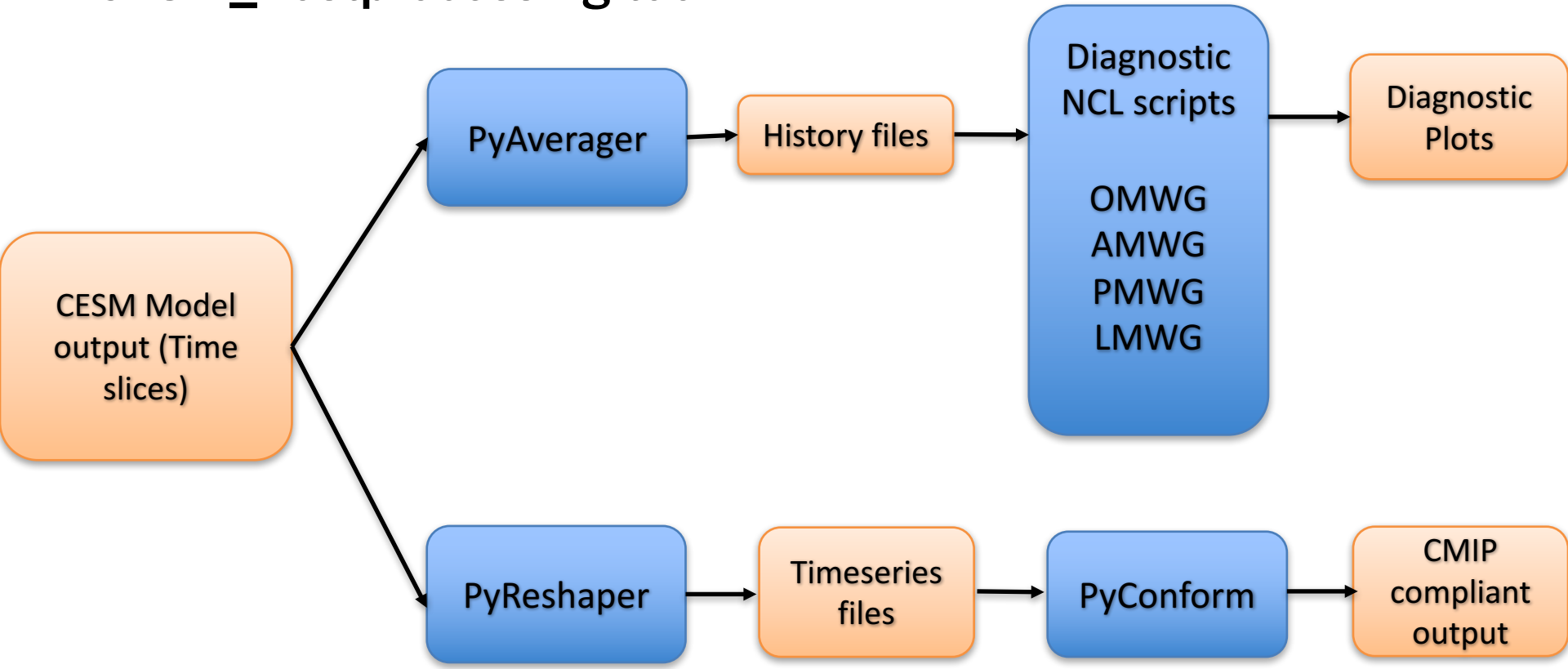
Other useful guides to utilities that can handle netCDF data include ARM's list of ARM-test
and the NOAA Geophysical Fluid Dynamics Laboratory guide to netCDF utilities.

Freely Available Software

- ANDX (ARM NetCDF Data eXtract) and ANAX (ARM NetCDF ASCII eXtract)
- ANTS (ARM NetCDF Tool Suite)
- ARGOS (interActive thRee-dimensional Graphics ObServatory)
- CDAT (Climate Data Analysis Tool)
- CDFconvert (Convert netCDF to RPN and GEMPAK Grids)
- cdfsync (network synchronization of netCDF files)
- CDO (Climate Data Operators)
- CIDS Tools
- CSIRO MATLAB/netCDF interface
- EPIC
- Excel Use
- EzGet
- FAN (File Array Notation)
- FERRET
- FIMEX (File Interpolation, Manipulation, and EXtraction)
- FWTools (GIS Binary Kit for Windows and Linux)
- GDAL (Geospatial Data Abstraction Library)
- GDL (GNU Data Language)
- Gfdnavi (Geophysical fluid data navigator)
- Gliderscope
- GMT (Generic Mapping Tools)
- Grace
- GrADS (Grid Analysis and Display System)
- Gri
- GXSM - Gnome X Scanning Microscopy project
- HDF (Hierarchical Data Format) interface
- HDF-EOS to netCDF converter
- HIPHOP (Handy IDL-Program for HDF-Output Plotting)

https://www.unidata.ucar.edu/software/netcdf/software.html

CESM_Postprocessing tool



Generated diagnostics

AMWG Diagnostics Package

b.e21.B1850.f09_g17.CMIP6-piControl.001
and
b.e21.B1850.f09_g17.CMIP6-piControl.001

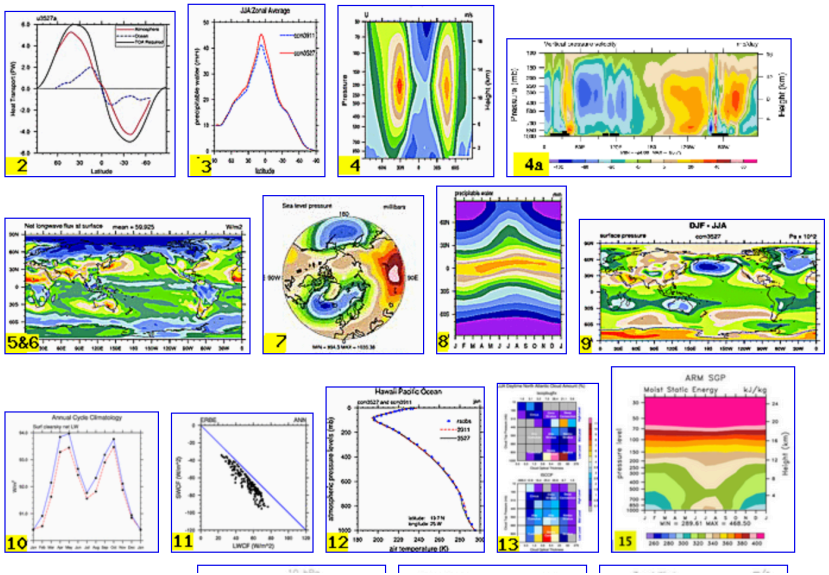
NCAR
National Center for Atmospheric Research
Boulder, Colorado

Plots Created
Tue Aug 28 11:32:34 2018

Set Description
1 Tables of ANN, DJF, MAM, JJA, SON, global and regional means and RMSE.
2 Line plots of annual implied northward transports.
3 Line plots of DJF, MAM, JJA, SON and ANN zonal means
4 Vertical contour plots of DJF, MAM, JJA, SON and ANN zonal means
4a Vertical (XZ) contour plots of DJF, MAM, JJA, SON and ANN meridional means
5 Horizontal contour plots of DJF, MAM, JJA, SON and ANN means
6 Horizontal vector plots of DJF, MAM, JJA, SON and ANN means
7 Polar contour and vector plots of DJF, MAM, JJA, SON and ANN means
8 Annual cycle contour plots of zonal means
9 Horizontal contour plots of DJF-JJA differences
10 Annual cycle line plots of global means
11 Pacific annual cycle, Scatter plot plots
12 Vertical profile plots from 17 selected stations
13 Cloud simulator plots
14 Taylor Diagram plots
15 Annual Cycles at Select Stations plots
16 Budget Terms at Select Locations plots

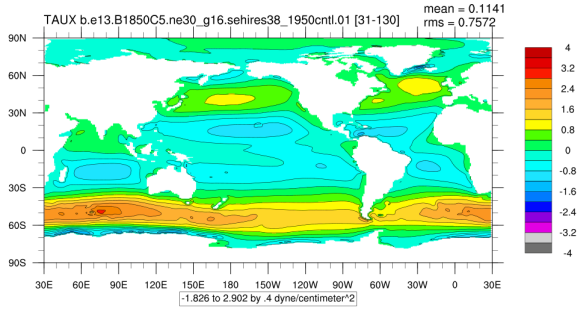
WACCM Set Description
1 Tables of regional min, max, means

Click on Plot Type

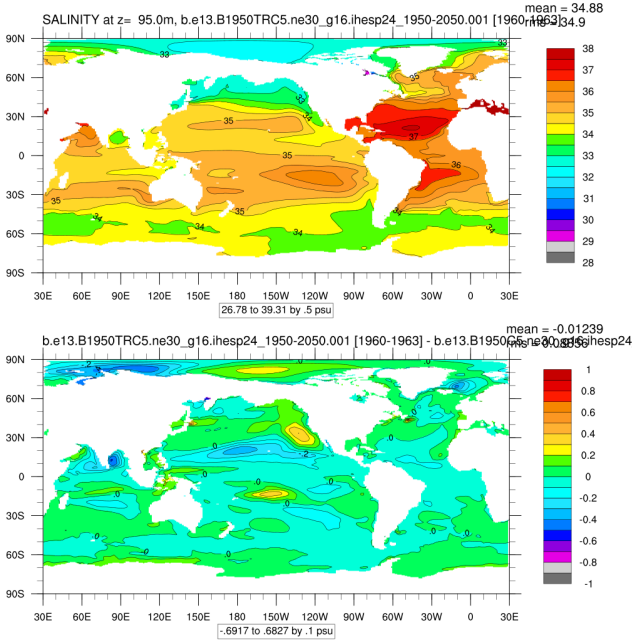


Diagnostic sets

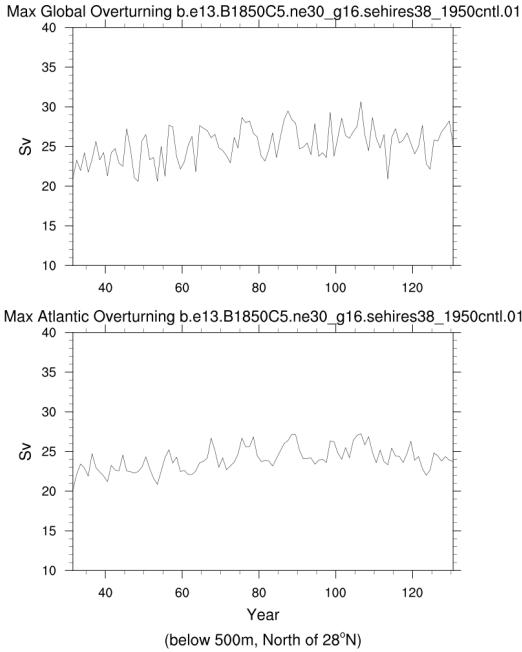
Model vs Observations



Model vs Control



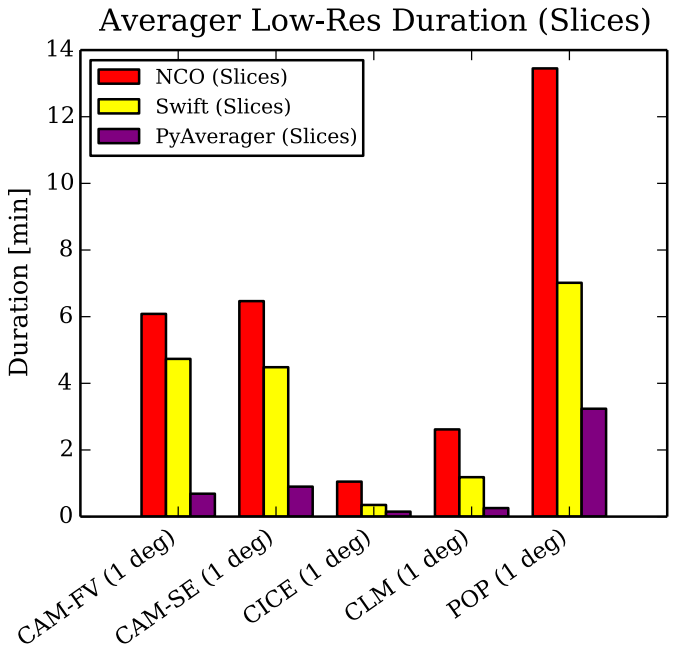
Model time series

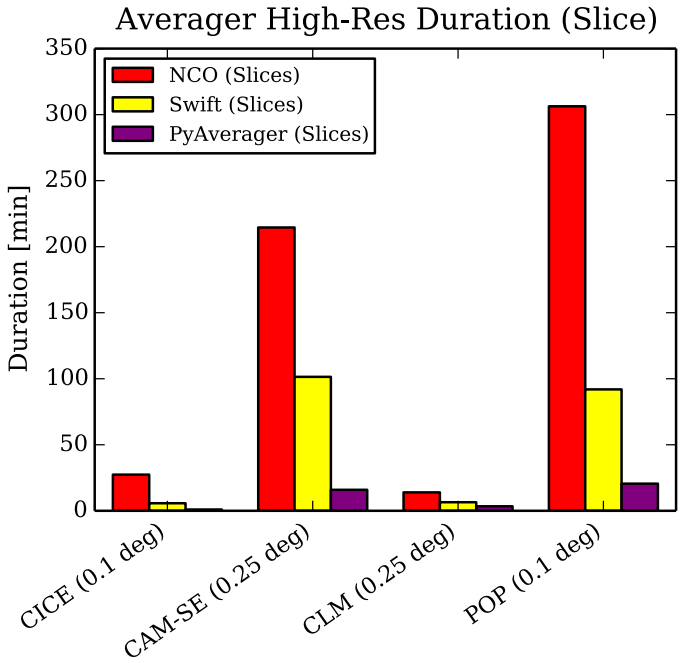


Some ocean diagnostics plots

Type of plot	Quantity
2D Surface flux fields	SENH_F, LWUP_F, EVAP_F, PREC_F
2D Surface fields	SSH, SST, etc
3D fields (Zonally-averaged)	TEMP, SALT, IAGE
Fields at various depth levels	TEMP, SALT, UVEL, VVEL, WVEL
Vector fields at various depth levels	velocity
MOC	

PyAverager performance





Sheri Mickelson[1] & Alice Bertini[2, NCAR]

POP 0.1deg grid = 15 times faster than NCO

Obtaining/installing the CESM diagnostics tool

https://github.com/abishekg7/CESM_postprocessing

- Forked from NCAR's github.
- Incorporates Ada-specific configuration created by Alper Altuntas
- Simplified installation process

Installation and Usage instructions

0. Load all necessary modules

```
module purge
ml NCL/6.6.2-foss-2018b
ml NCO/4.7.9-foss-2018b
ml netCDF/4.6.1-foss-2018b-cdf5
ml Python/2.7.15-foss-2018b
```

1. Clone CESM_postprocessing

```
git clone https://github.com/abishekg7/CESM_postprocessing.git
cd CESM_postprocessing
```

2. Install virtual environment:

```
./create_python_env -machine ada
```

Creating a post-processing case on Ada

1. Activate the PP virtual environment

```
ml purge
ml Miniconda2/4.3.21
ml Python/2.7.15-foss-2018b
export POSTPROCESS_PATH=/scratch/training/CESM_post/CESM_postprocessing
source activate $POSTPROCESS_PATH/cesm-env2
```

2. Create a post-processing case directory in your scratch directory

```
create_postprocess -case [your-case-directory]
```

Exercise: Try above commands on Ada

Post-processing workflow

1. Edit configuration files
   - env_postprocess.xml
   - env_diags_ocn.xml, env_diags_atm.xml, etc
2. Edit job submission scripts (ocn_averages, ocn_diagnostics, etc)
   - Change project account, num_cores, logging level, etc
3. Generate averaged files

   bsub < ocn_averages
4. Generate diagnostics

   bsub < ocn_diagnostics

Variables in env_postprocess.xml

Variable	Purpose
CASEROOT	Location of caseroot. Same as PP_CASE_PATH for standalone postprocessing
PP_CASE_PATH	Disk location of postprocessing case directory
CASE	CESM Case name
DOUT_S_ROOT	CESM model output directory. Input for post-processing
<COMP>_GRID	String specifying grid for component <COMP>
GENERATE_TIMESERIES	If True, converts history to timeseries files
GENERATE_AVGS_<COMP>	If True, calls averaging script for component <COMP>
GENERATE_DIAGS_<COMP>	If True, calls diagnostics script for component <COMP>

Sample values for env_postprocess.xml

Variable	Purpose
CASEROOT	/scratch/training/CESM_post/pp_cases/pp_control
PP_CASE_PATH	/scratch/training/CESM_post/pp_cases/pp_control
CASE	b.e13.B1950C5.ne30_g16.ihesp24_1950cntl.001
DOUT_S_ROOT	/scratch/training/CESM_post/datasets/b.e13.B1950C5.ne30_g16.ihesp24_1950cntl.001
ATM_GRID	ne30
OCN_GRID	gx1v6
ICE_GRID	gx1v6
LND_GRID	ne30

Grid descriptions

http://www.cesm.ucar.edu/models/cesm1.0/cesm_doc_1_0_4/a3714.html

Grid descriptor	Type of grid
1.9x2.5 or f19	Regular lon/lat finite volume grids of approximately 1.9 and 2.5 degree lon and lat respectively.
T85	Spectral lon/lat grids with 85 as the spectral truncation value for the resolution
ne30np4	Cubed sphere resolutions where X and Y are integers. The short name is generally ne[X]
pt1	Single pt grid
gx1v6 or g16	Displaced pole grid of approximately 1 degree resolution. 6 denotes the grid version.
tx0.1v2	Tripole grid of approx 0.1 degree resolution. 2 denotes the grid version.

Variables in env_diags_ocn.xml

Variable	Purpose
OCNDIAG_DIAGOBSROOT	/scratch/training/CESM_post/obs_root
OCNDIAG_TAVGDIR	$PP_CASE_PATH/ocn_out/climo.$OCNDIAG_YEAR0.$OCNDIAG_YEAR1
OCNDIAG_WORKDIR	$PP_CASE_PATH/ocn_out/diag_work.$OCNDIAG_YEAR0-$OCNDIAG_YEAR1
OCNDIAG_netcdf_format	netcdfLarge (64-bit)
OCNDIAG_MODEL_VS_OBS	TRUE
OCNDIAG_MODEL_VS_CONTROL	FALSE
OCNDIAG_MODEL_TIMESERIES	TRUE

After averaging step (check $OCNDIAG_WORKDIR)

1. 12 Climatology files (averaged for each month)
   - **$CASE.$YEAR0-$YEAR1.<MONTH>_climo.nc**
2. Yearly-averaged files for every year
   - **$CASE.$YEAR0.nc**
3. Time average (Single file)
   - **tavg. $YEAR0-$YEAR1.nc**
4. Monthly average (Concatenation of the climatology files)
   - **mavg. $YEAR0-$YEAR1.nc**

Exercise – generating averages

1. Create a new postprocessing case for the transient case

2. Copy env_postprocess.xml and env_diags_ocn.xml from the existing control case configuration at /scratch/training/CESM_post/pp_cases/pp_control and edit for the transient case

3. Submit ocn_averages

Short break!
(15 minutes)

Submit diagnostics

1. bsub < ocn_diagnostics

Generated ocean diagnostics

CESM Ocean Diagnostics Plots

CESM Version: ihesp24
Diagnostics Generated by: agopal
Diagnostics Generated on: 2020-04-08 17:43:10
Case Name: b.e13.B1950C5.ne30_g16.ihesp24_1950cntl.001
Years: 35 - 38
Timeseries Years: 35 - 38

- MODEL_VS_OBS
- MODEL_VS_OBS_ECOSYS - no plots available
- MODEL_VS_CONTROL - no plots available
- MODEL_TIMESERIES

NCAR

CESM Ocean Diagnostics Plots Model vs. Observations

CESM Version: ihesp24
Diagnostics Generated by: agopal
Diagnostics Generated on: 2020-04-08 17:43:12
Case Name: b.e13.B1950C5.ne30_g16.ihesp24_1950cntl.001
Years: 35 - 38

2D Surface Flux Fields

Surface Fluxes (Lat, Lon)

SHF_TOTAL SHF_QSW MELTH_F SENH_F LWUP_F LWDN_F QFLUX
SFWF_TOTAL EVAP_F PREC_F SNOW_F MELT_F SALT_F ROFF_F
TAUX TAUY CURL

Global Zonal Average

SHF_GLO_za SHF_QSW_GLO_za MELTH_F_GLO_za SENH_F_GLO_za LWUP_F_GLO_za LWDN_F_GLO_za QFLUX_GLO_za
SFWF_GLO_za EVAP_F_GLO_za PREC_F_GLO_za SNOW_F_GLO_za MELT_F_GLO_za SALT_F_GLO_za ROFF_F_GLO_za

2D Surface Fields

2D Fields (Lat, Lon)

SSH HBLT HMXL DIA_DEPTH TLT INT_DEPTH
SU SV BSF

Global Zonal Average

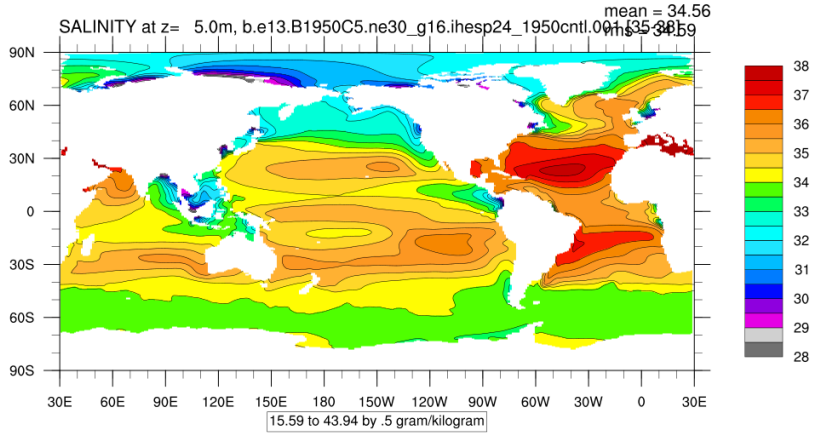
SSH_GLO_za HBLT_GLO_za HMXL_GLO_za DIA_DEPTH_GLO_za TLT_GLO_za INT_DEPTH_GLO_za

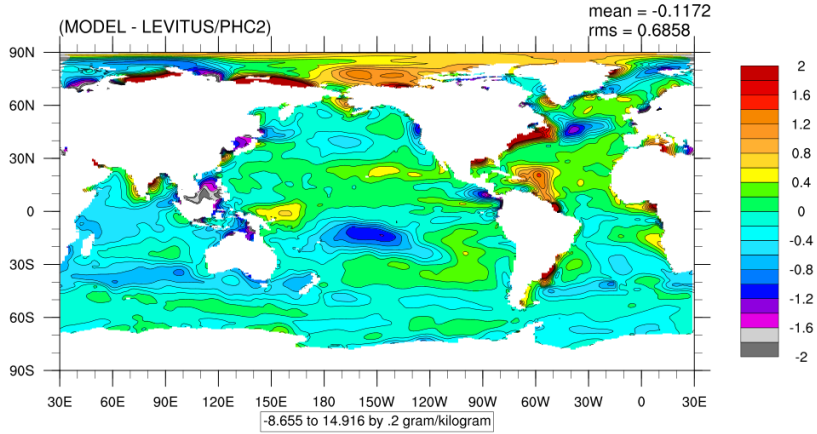
3D Fields, Zonally Averaged

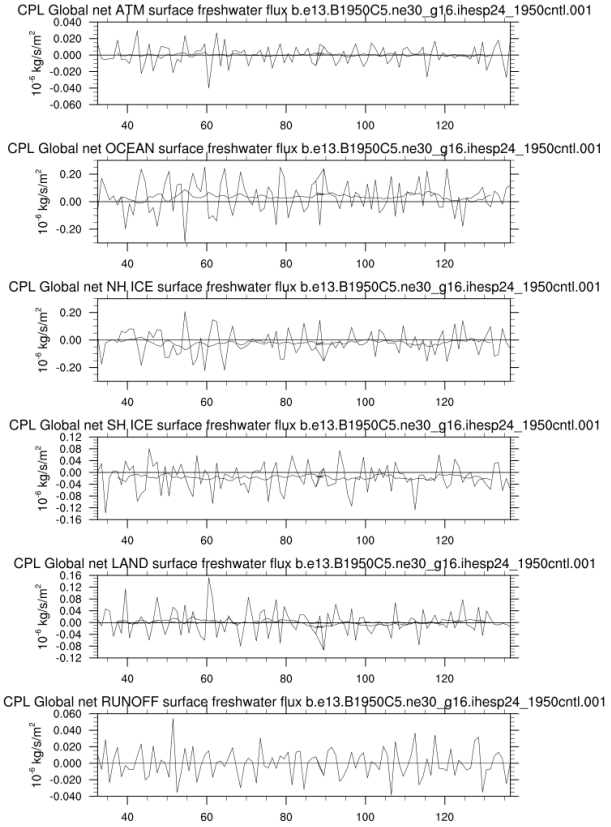
3D Fields, Zonally-Averaged

Global	TEMP_GLO_za	SALT_GLO_za	IAGE_GLO_za	KAPPA_ISOP_GLO_za
Atlantic	TEMP_ATL_za	SALT_ATL_za	IAGE_ATL_za	KAPPA_ISOP_ATL_za

Generated ocean diagnostics







Exercise – generating diagnostics

1. Turn on the correct diagnostic sets in env_diags_ocn.xml

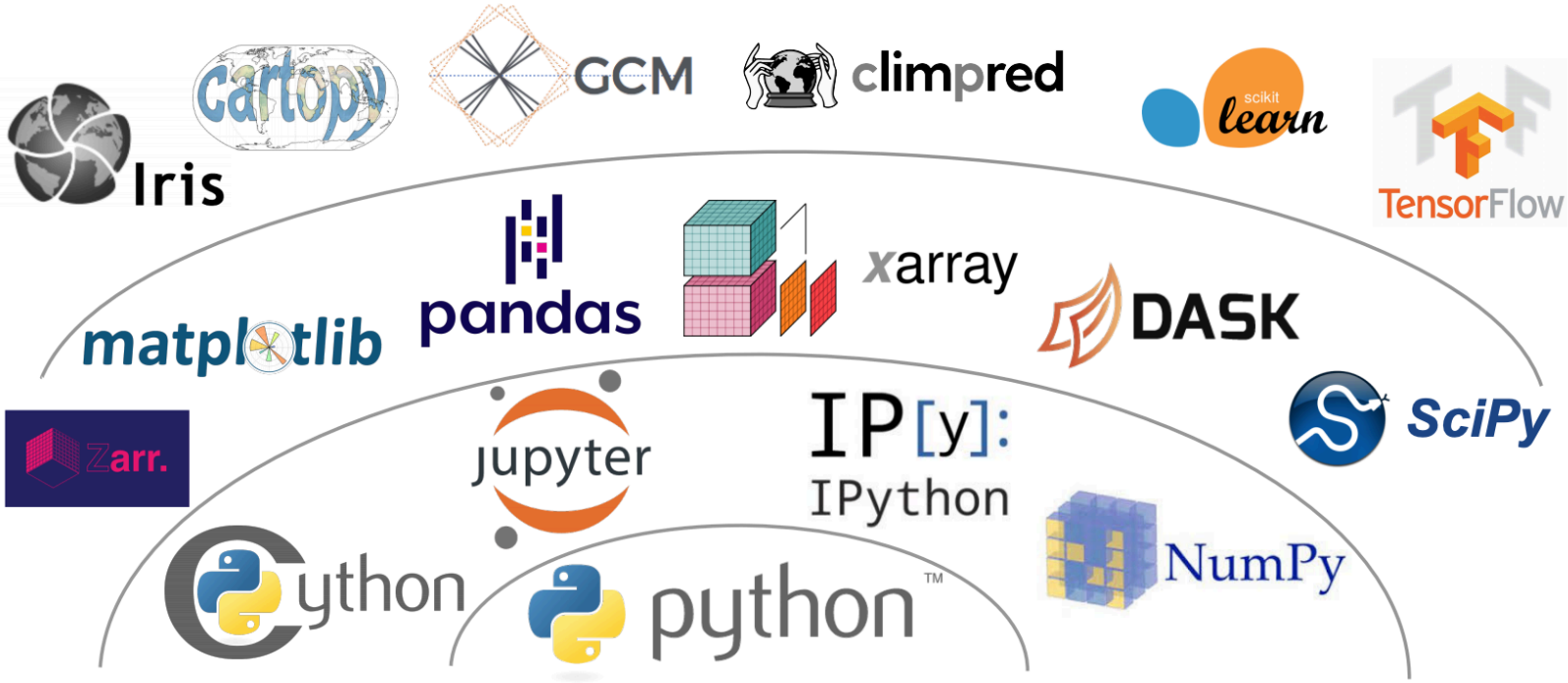
2. Check the ocn_diagnostics script for correctness

3. Submit ocn_diagnostics

Limitations of the current diagnostics tool

- Patchwork of many different components. Harder to locate centralized help/documentation
- Adding new diagnostic sets is a challenge
- Porting to a new machine can be tricky

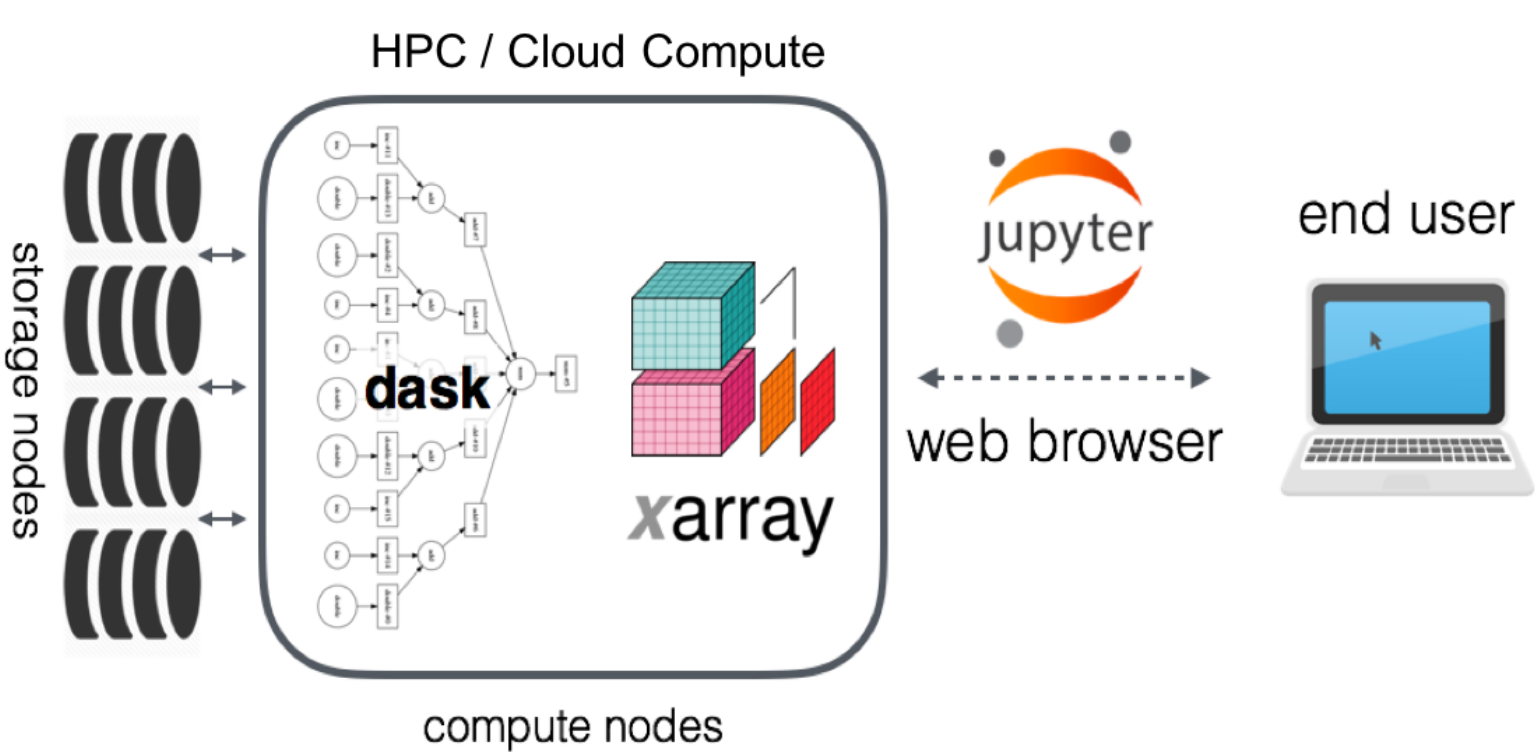
Pangeo framework



Ryan Abernathey

Pangeo

https://pangeo.io/architecture.html



What is xarray

- An extension of the pandas library to work with labelled, N-dimensional arrays
- 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

```
[2]: import xarray as xr
     ds = xr.open_dataset('/scratch/training/CESM_post/datasets/b.e13.B1950C5.ne30_g16.ihesp24_1
     ds
```

[2]: xarray.Dataset

▸ Dimensions: (d2: 2, **lat_aux_grid**: 395, moc_comp: 3, **moc_z**: 61, nlat: 384, nlon: 320, **time**: 1, transport_comp: 5, transport_reg: 2, **z_t**: 60, **z_t_150m**: 15, **z_w**: 60, **z_w_bot**: 60, **z_w_top**: 60)

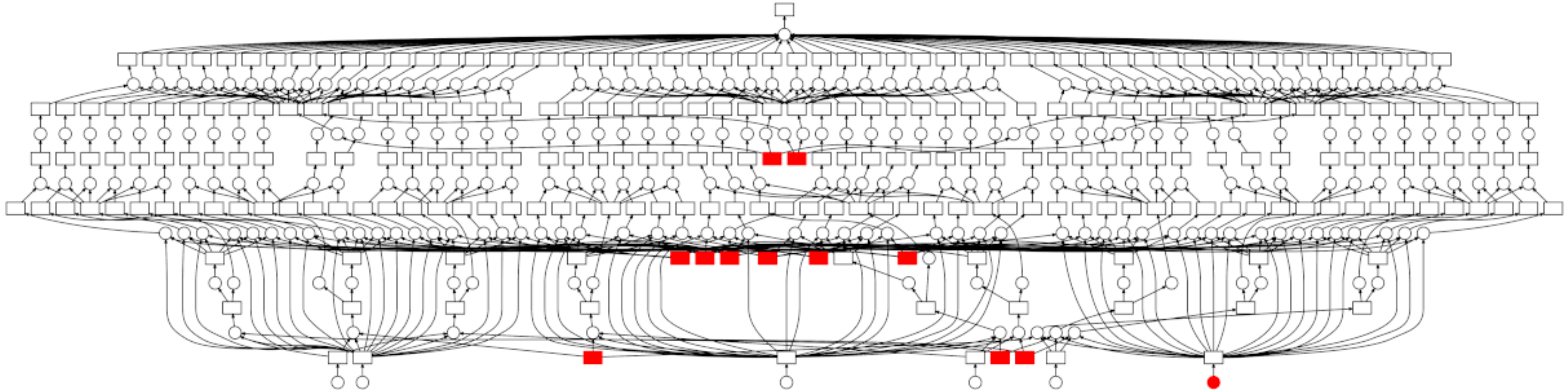
▾ Coordinates:

transport_comp...	(transport_comp)	|S256	...
transport_regions	(transport_reg)	|S256	...
time	(time)	object	0038-05-01 00:00:00
z_t	(z_t)	float32	500.0 1500.0 ... 512502.8 537500.0
z_t_150m	(z_t_150m)	float32	500.0 1500.0 ... 13500.0 14500.0
z_w	(z_w)	float32	0.0 1000.0 ... 500004.7 525000.94
z_w_top	(z_w_top)	float32	0.0 1000.0 ... 500004.7 525000.94
z_w_bot	(z_w_bot)	float32	1000.0 2000.0 ... 549999.06
lat_aux_grid	(lat_aux_grid)	float32	-79.48815 -78.952896 ... 90.0
moc_z	(moc_z)	float32	0.0 1000.0 ... 525000.94 549999.06
ULONG	(nlat, nlon)	float64	...
ULAT	(nlat, nlon)	float64	...
TLONG	(nlat, nlon)	float64	...
TLAT	(nlat, nlon)	float64	...

▸ Data variables: (113)

▸ Attributes: (11)

Dask task graph

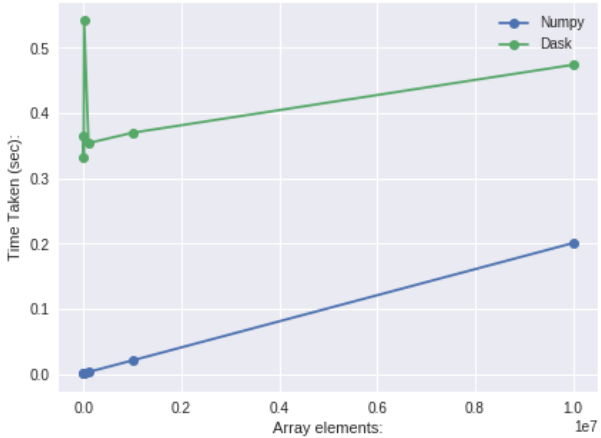


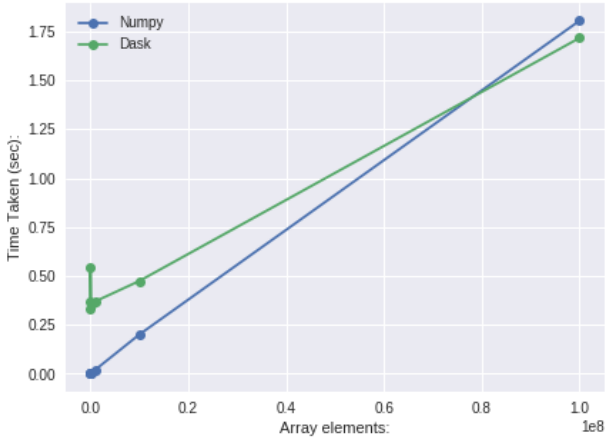
https://towardsdatascience.com/speeding-up-your-algorithms-part-4-dask-7c6ed79994ef

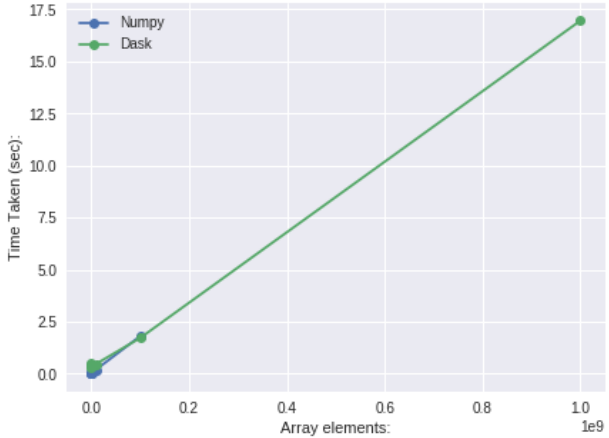
Dask vs Numpy

- Numpy is faster than Dask for a smaller problem size
- For larger problems, Dask achieves better scalability
- Numpy cannot load very large arrays, whereas Dask works just fine

https://towardsdatascience.com/speeding-up-your-algorithms-part-4-dask-7c6ed79994ef

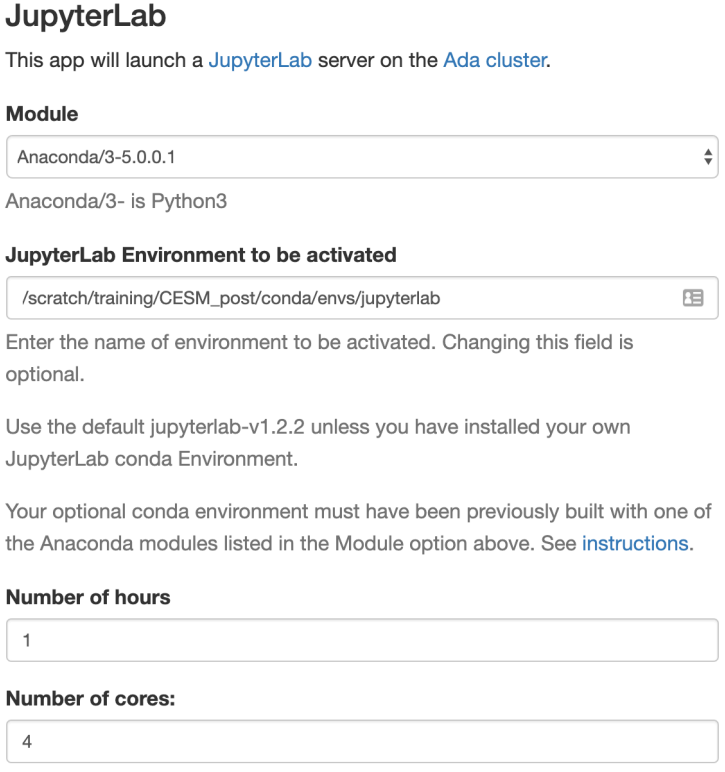






Launch JupyterLab notebook

- Go to https://portal.hprc.tamu.edu/
- Choose Ada, then Interactive Apps -> JupyterLab from the top pane
- Enter path to JupyterLab environment **/scratch/training/CESM_post/conda/envs/jupyterlab**
- Request 1 hour on 4 cores, 1 GB memory per core (4 GB in total)
- Click Launch

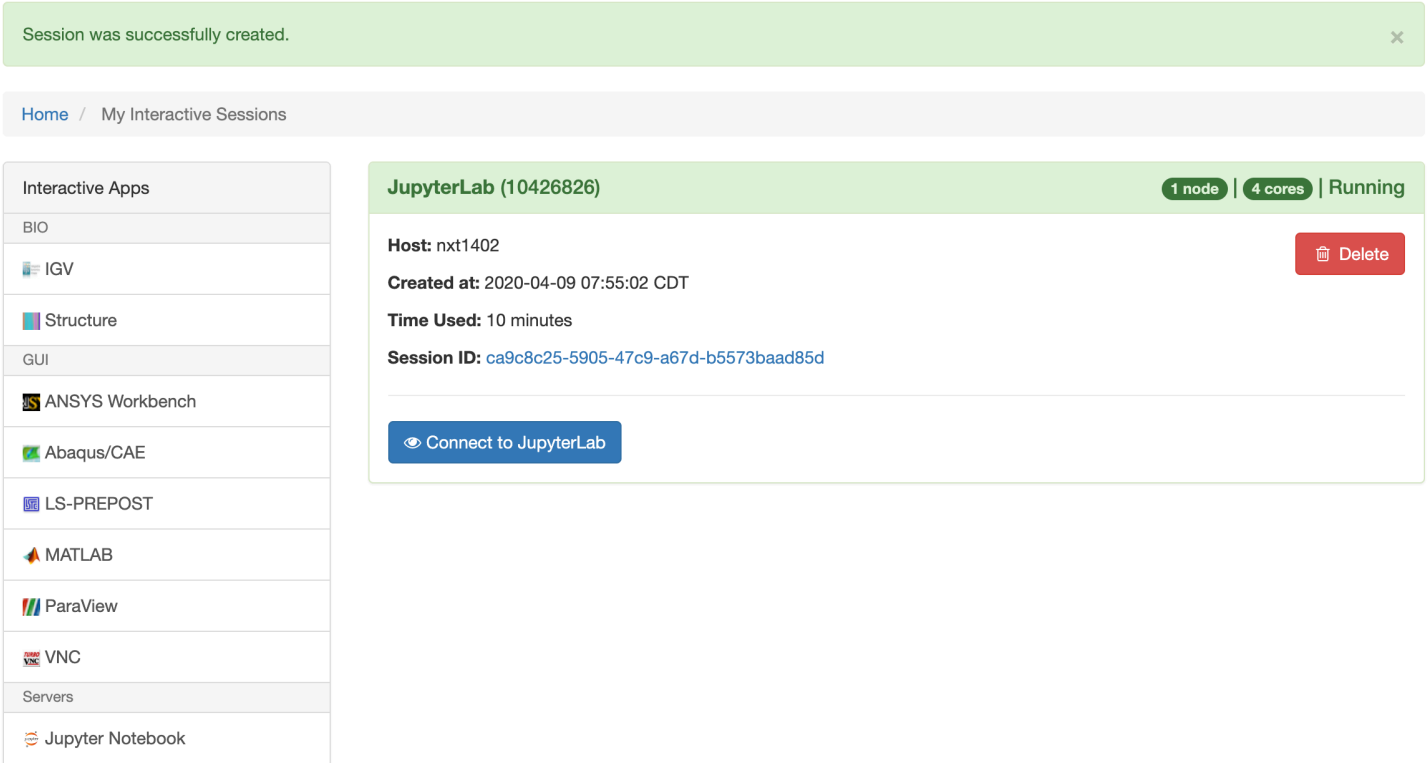


Download tutorial notebooks

- ssh <username>@ada.tamu.edu
- cd into your scratch directory
- Clone the notebook repository from github

  git clone https://github.com/abishekg7/pangeo_binders.git

Launch JupyterLab notebook



Additional resources

- CESM diagnostics tool tutorials
  - http://www.cesm.ucar.edu/events/tutorials/2019/files/Practical3-phillips.pdf
  - http://www.acacia.ucar.edu/events/2019/ctsm/files/practical21-oleson.pdf
  - http://www.cesm.ucar.edu/events/workshops/ws.2016/presentations/sewg/bertini.pdf
- GeoCAT
  - https://geocat.ucar.edu/pages/software.html
- Pangeo forums
  - http://discourse.pangeo.io/

Acknowledgements

- Fred Castruccio and Alper Altuntas, NCAR
- Sanjiv Ramachandran and Dapeng Li, iHESP
- The HPRC team

Questions?