



Empowering Transformational Science

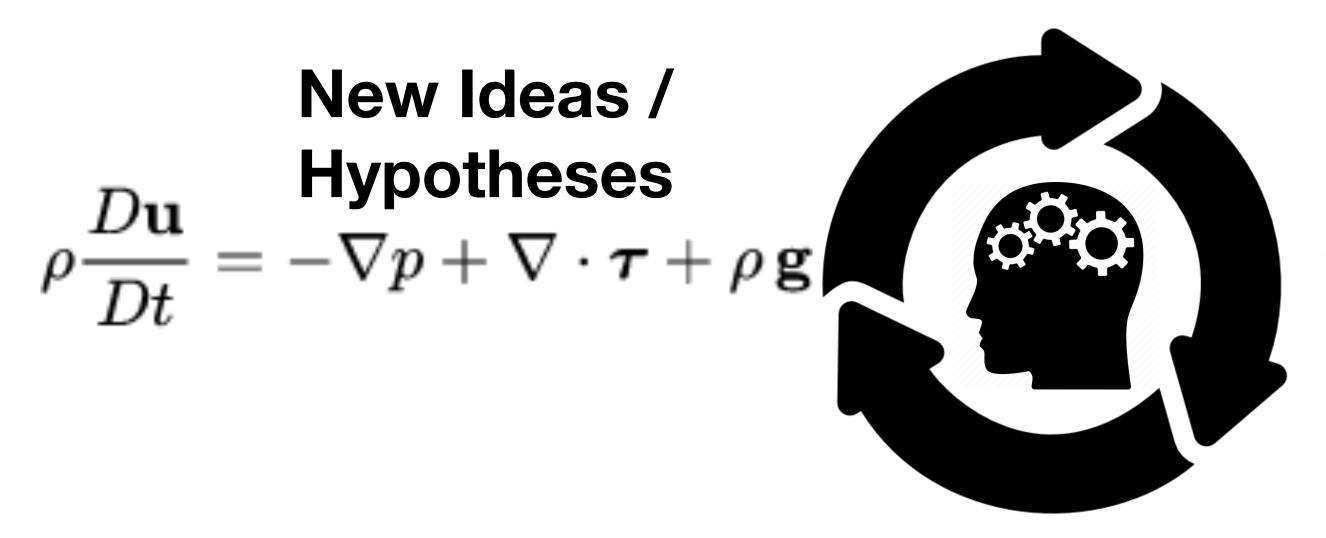
Chelle Gentemann (Farallon Institute) twitter: <u>occupations</u>
Ryan Abernathey (Columbia / LDEO) twitter: <u>occupations</u>
Aimee Barciauskas (Development Seed) twitter: <u>occupations</u>
(there are lots of links in this presentation! click away!)



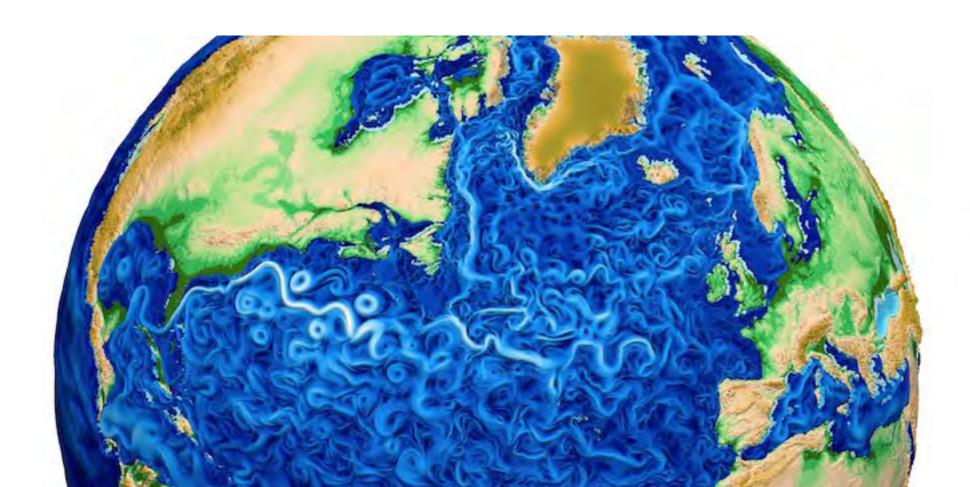




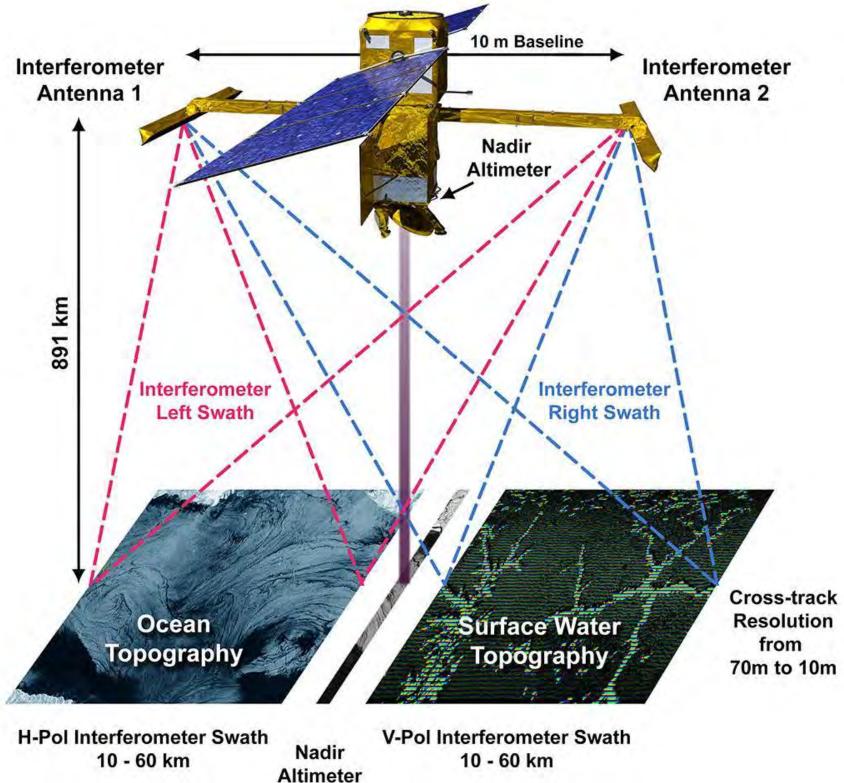
What Drives Progress in Earth System Science?



New Simulations



New Observations



Path





What impacts the velocity of progress? Data, Software, & Compute

Data: time to find, access, clean, & format data for analysis

Software: what tools are easily available?

Compute: access to compute == speed of results

80%
Data Preparation
(download, clean, & organize files)

10%
Batch
Processing

10%
Think about science

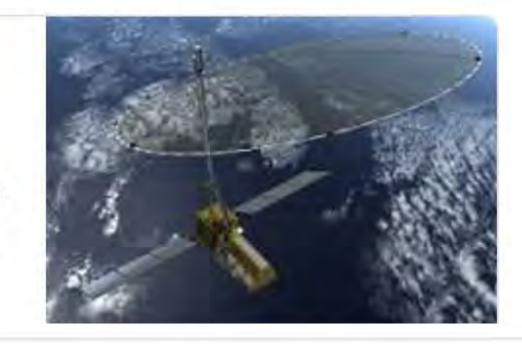




Traditional methods of data access cannot leverage large volumes of data

US\$1.5 billion

With a total cost estimated at US\$1.5 billion, NISAR is likely to be the world's most expensive Earth-imaging satellite.



en.wikipedia.org > wiki > NISAR_(satellite) *

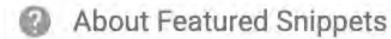
NISAR (satellite) - Wikipedia

140 petabytes

As Dobson notes, NISAR is expected to generate a tremendous volume of data over its scheduled three-year mission — as much as 140 petabytes (PB).

asf.alaska.edu → wp-content → uploads → 2019/06 → 201... ▼ PDF

Getting Ready for NISAR - Alaska Satellite Facility



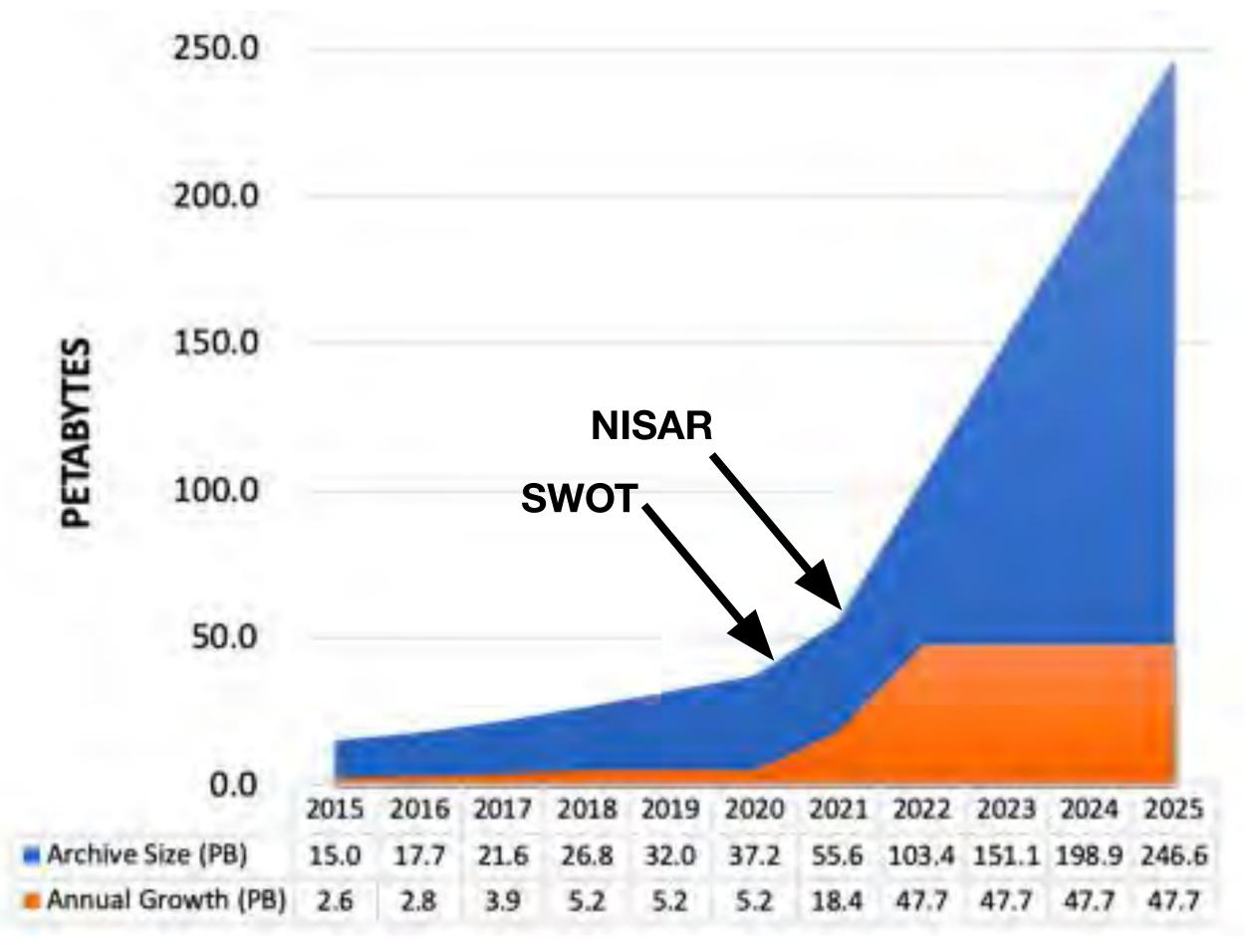




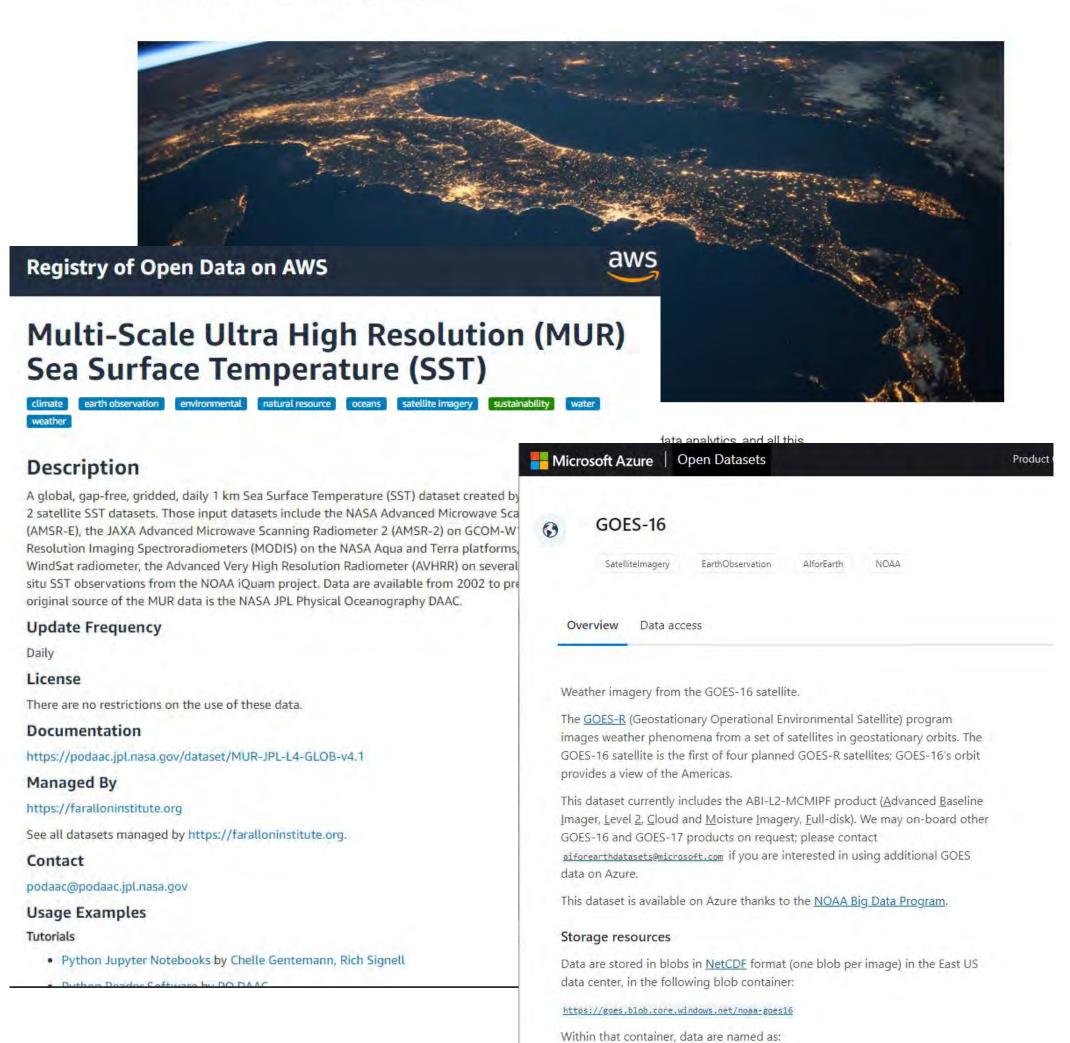


Data, Software, Compute New climate model data now in Google Public Datasets

DATA ANALYTICS



https://earthdata.nasa.gov/eosdis/cloud-evolution



[product]/[year]/[day]/[hour]/[filename]





Analytics Optimized Data Store (AODS)

a few examples of AODS formats







Current method -

NetCDF files - organized into 'reasonable' data sizes per file, usually by orbit, granule, or day. Filename has information about date, sensor, version. Reading usually involved calculating the filename, opening, reading, processing, closing.

Analytics Optimized Data Store (one example of many different formats)

Zarr - makes large datasets easily accessible to distributed computing. Original data is stored in directories each having chunked data corresponding to dataset dimensions. Metadata is read by zarr libraries to read only the chunks necessary to complete a subsetting request.

Technology advances -

Lazy loading - also known as asynchronous loading - defer initialization of an object until the point at which it is needed. Developed for webpages. Delays reading data until needed for compute.

Advanced OSS libraries:

Xarray - library for analyzing multi-dimensional arrays, lazy loading.

Dask - able to break a large computational problems into a network of smaller problems for distribution across multiple processors

Intake - lightweight set of tools for loading and sharing data in data science projects

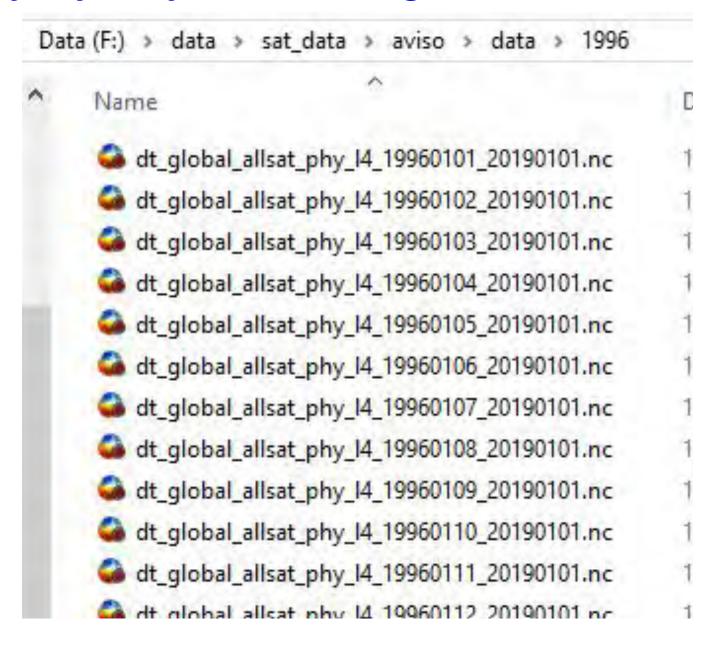




What does a data store look like?

Netcof

Organized so that each file can fit into RAM, usually by day, orbit, or granules



Zarr

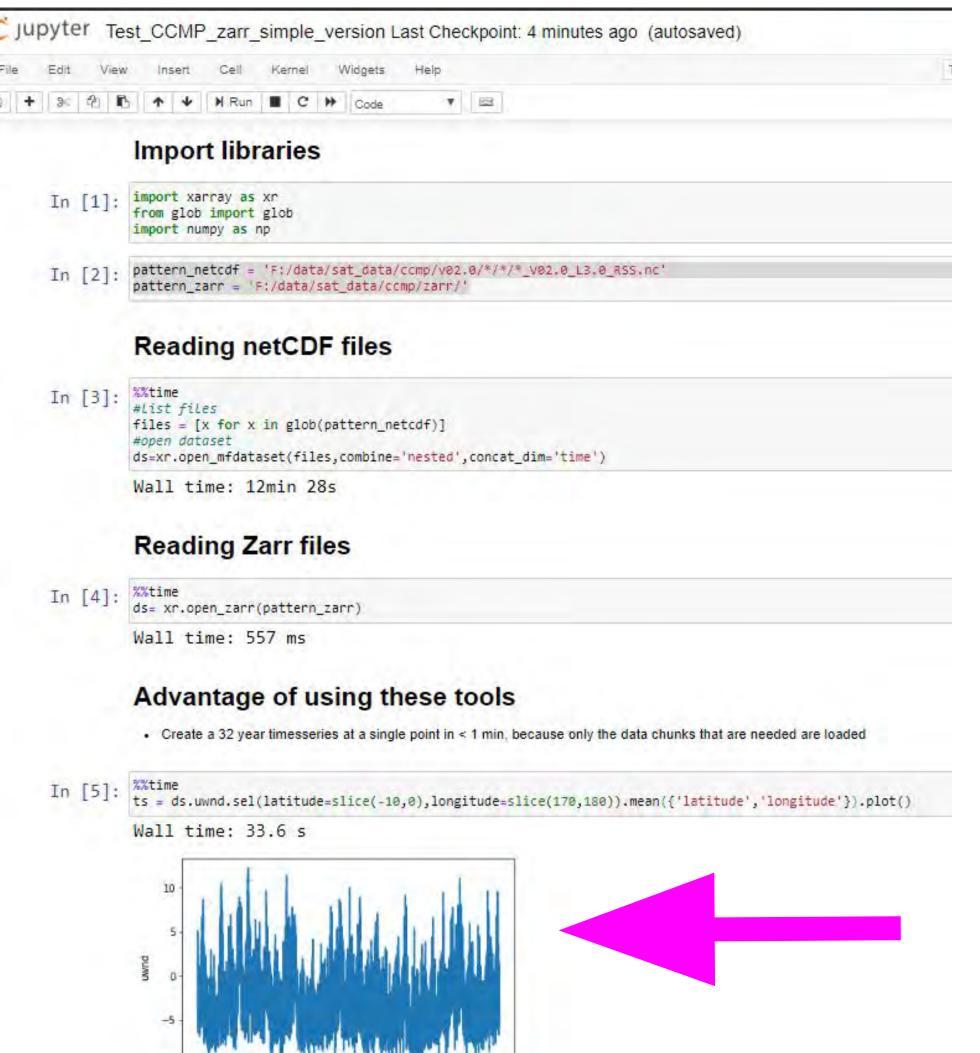
organization and format invisible to user, data accessed by metadata

Dat	ta (F:) > data :	sat_data	>	aviso	>	zarr	>	sla
^	Name	^						- 1:
	zarray							
	.zattrs							
	0.0.0							
	0.0.1							
	0.0.2							
	0.0.3							
	0.0.4							
	0.0.5							
	0.0.6							
	F3 007							





How to access data?



Modern software tools use lazy loading to access large datasets



My version of lazy loading before I knew python - on bedrest, pregnant with twins

Reading in netCDF data: 13 minutes (depends on computer)

- 1 user creates list of filenames
- 2 access dataset by reading the metadata distributed through files

Reading in Zarr data: 0.1 seconds (metadata consolidated)

1 - access dataset by reading the consolidated metadata

STOP ----- THIS IS DIFFERENT ------

- 1 line of code to access a 32-year, global, 25km dataset
- 1 line of code to select a region, calculate mean, & plot time series in LESS than 1 minute

https://nbviewer.jupyter.org/github/cgentemann/Biophysical/blob/master/Test CCMP zarr simple version.ipynb





Data, Software, Compute



Inspiration: Stephan Hoyer, Jake Vanderplas (SciPy 2015)





Read CMIP6 data from Google Cloud using intake

500TB!!!



The CMIP6 data is a huge collection of different experiements. Access to these data uses the intake-esm library which you then use the catalog to select specific variables, experiments, or activities. (Note: intake-esm is quite news and experimental.) There are some great tutorials here and here.

More information on CMIP6 is here and variable names here

A nice introduction is here

The Pangeo catalog listing is here

```
col = intake.open_esm_datastore("https://raw.githubusercontent.com/NCAR/intake-esm-datastore/master/catalogs/pangeo-cmip6.json")
    CPU times: user 898 ms, sys: 156 ms, total: 1.05 s
71: pangeo-cmip6-ESM Collection with 267459 entries:
            > 15 activity_id(s)
           > 33 institution_id(s)
           > 70 source_id(s)
           > 102 experiment id(s)
           > 140 member_id(s)
           > 29 table_id(s)
           > 369 variable_id(s)
           > 10 grid_label(s)
           > 267459 zstore(s)
           > 60 dcpp_init_year(s)
```

Search the collection for historical, monthly, air temperature, for one realization

You can use the variable id (link given above) to search for different parameters, change the table id from atmospheric monthly to ocean monthly, 3hrly data etc. More information on what you can search for is in this tutorial

```
cat_cmip = col.search(experiment_id=['ssp585', 'historical'], # pick the 'historical' forcing experiment
                                             # choose to look at atmospheric variables (A) saved at monthly resolution (mon)
                 table_id='Amon',
                 variable_id='tas',
                                             # choose to look at near-surface air temperature (tas) as our variable
                 member_id = 'rlilp1f1') # arbitrarily pick one realization for each model (i.e. just one set of initial conditions)
cat_cmip
```

[8]: pangeo-cmip6-ESM Collection with 67 entries:

- > 2 activity_id(s)
- > 27 institution_id(s)
- > 42 source_id(s)

> 2 experiment_id(s)

Intake catalogues can significantly reduce friction (or barriers to entry) caused by figuring out how to access data stores

A powerful way to provide access for non-experts

Maintains all metadata

Users can easily build OSS libraries to harmonize data

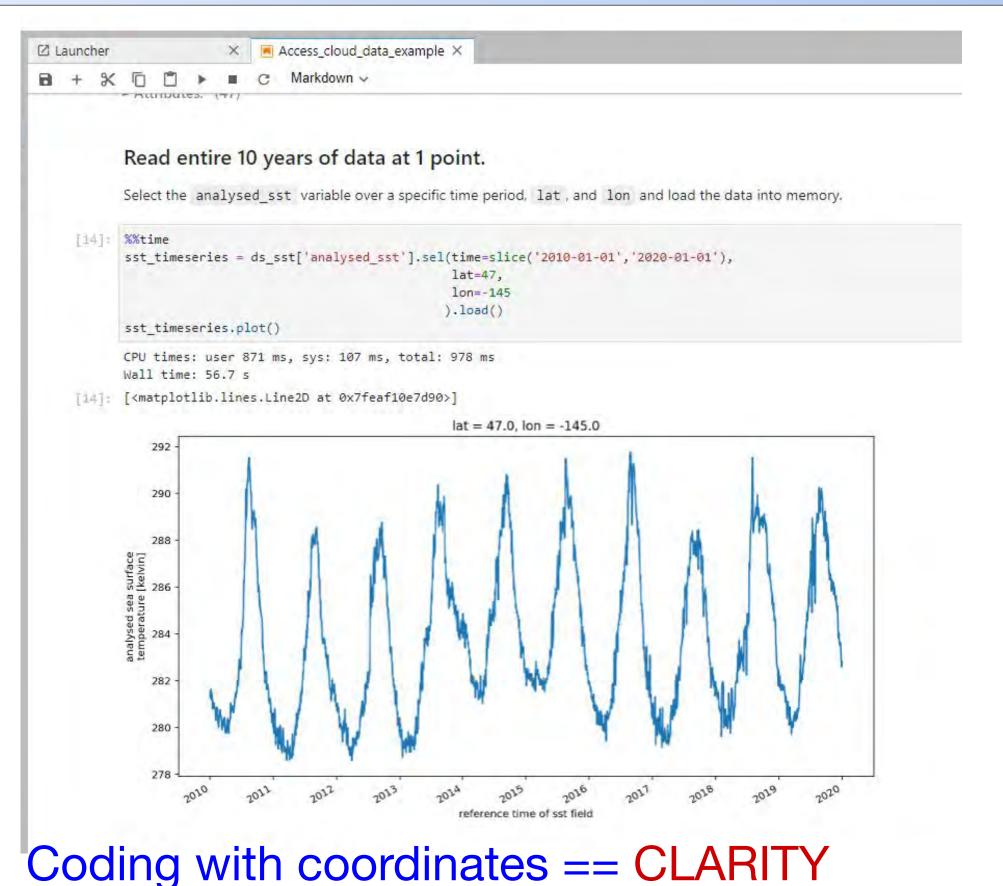




https://github.com/pangeo-gallery/osm2020tutorial







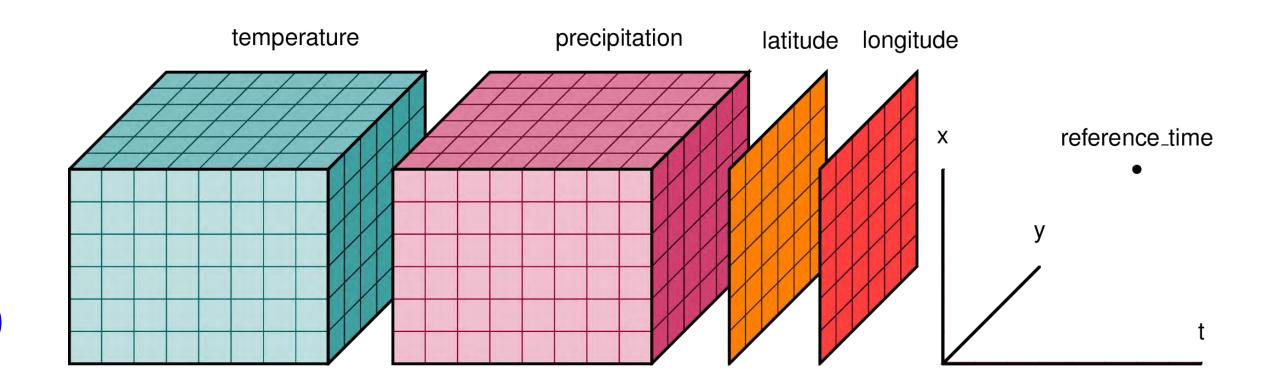
Xarray

@xarray_dev





Xarray introduces labels in the form of dimensions, coordinates and attributes on top of raw NumPy-like multidimensional arrays, which allows for a more intuitive, more concise, and **less error-prone** developer experience.



Make a timeseries:

data.sel(latitude=10,longitude=0,method='nearest').plot()

Regrid data for multivariate analysis: data_regrid = data.interp_like(other_data)

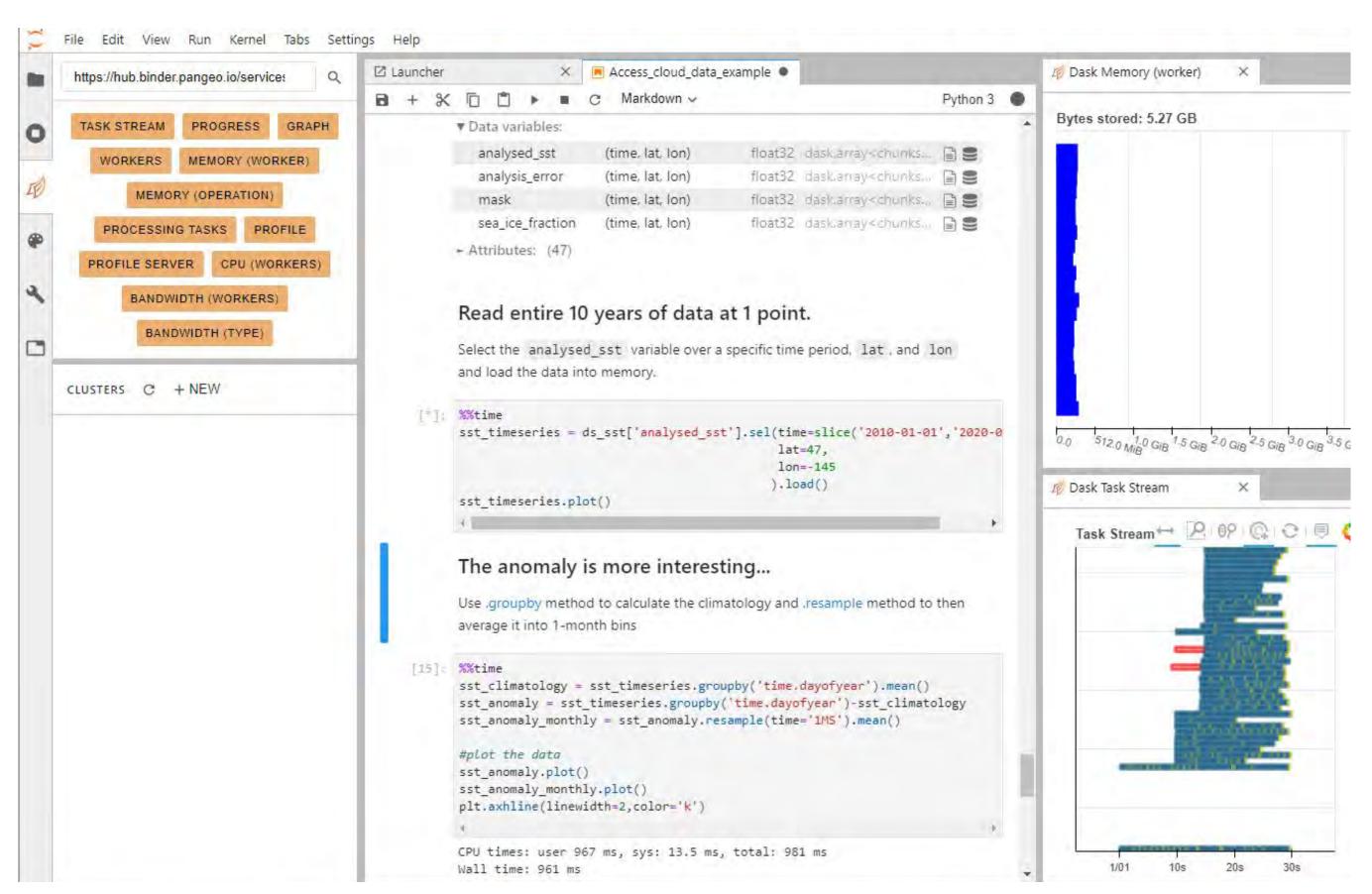
https://github.com/pangeo-gallery/osm2020tutorial







@dask_dev



VIJMFCDCUS

OPEN CODE = BETTER SCIENCE



Dask is a flexible library for parallel computing in Python.

Xarray integrates with Dask to support parallel computations and streaming computation on datasets that don't fit into memory. When you are using Xarray, you are likely using Dask without even realizing it.

The Pangeo binder and jupyterhub use <u>Dask</u> <u>Gateway</u> to manage access to the Dask clusters & kubernetes.

Cluster performance visualization using the Dask viewers: memory use, profile, CPU, etc.





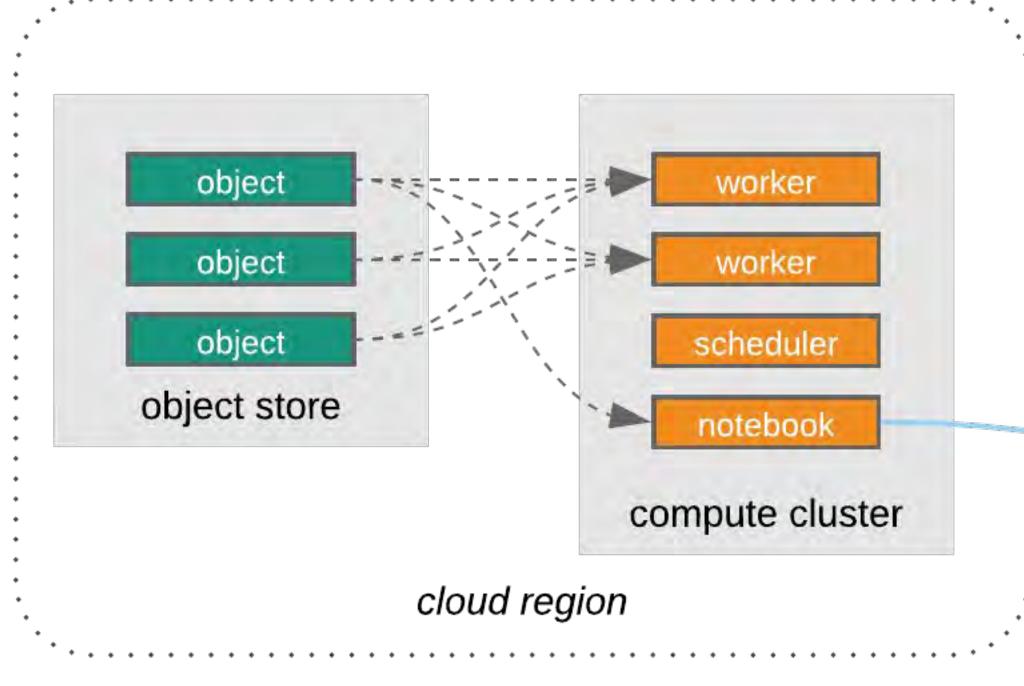
Data, Software, Compute

Analytics Optimized Data Store (AODS)









Scalable Parallel
Computing Frameworks



figures



Data Consumer's





Data Provider's









Policies



EXPLORE DEVELOP ABOUT PRICING BLOG

CLOUD API

ATELLITE IMAGERY

Agency driven solutions

Cloud Operations Administrator

Thematic Applications

Processing tutorials

Source



heterogeneous nature of the data, which a

resolutions, coverages, and processing leve

and immediate need for improved data sha

MAAP is addressing these community need

Enabling researchers to easily discover,

· Harmonizing satellite, airborne, and gro

Developing tools for repeatable and sha

data generation.

NASA missions and validation/calibratio

ESA CloudToolbox The ESA CloudToolbox is a Virtual Machine (VM) that offers a flexible amount of CPUs, RAM and dedicated storage, tailored to user needs and type of machine required. When needed, users can request upgrades of the configuration (for example, asking more processing power) at any time, compatibly with the Cloud infrastructure constraints. A pre-built VM template offers ready-to-use machines for SAR Interferometric processing or generic EO data processing. However, besides free and licensed software tools (e.g. Sentinel-1 toolbox, NEST, GAMMA, Matlab, etc) that can be installed on the machines, users may request installation of additional tools. Create a CloudToolbox To create your own CloudToolbox: • Access the cloud dashboard (see Cloud Dashboard)

SENTINEL Hub

Create Virtual Machine

Set the Virtual Machine name (e.g 'my esa toolbox')

· Select the ESA Cloud Toolbox template

· Wait for the VM to be deployed

Get the <ESA CloudToolbox IP>

· Click on Create

to create a new Virtual Machine

my esa toolbox

@esa ESA Cloud Toolbox





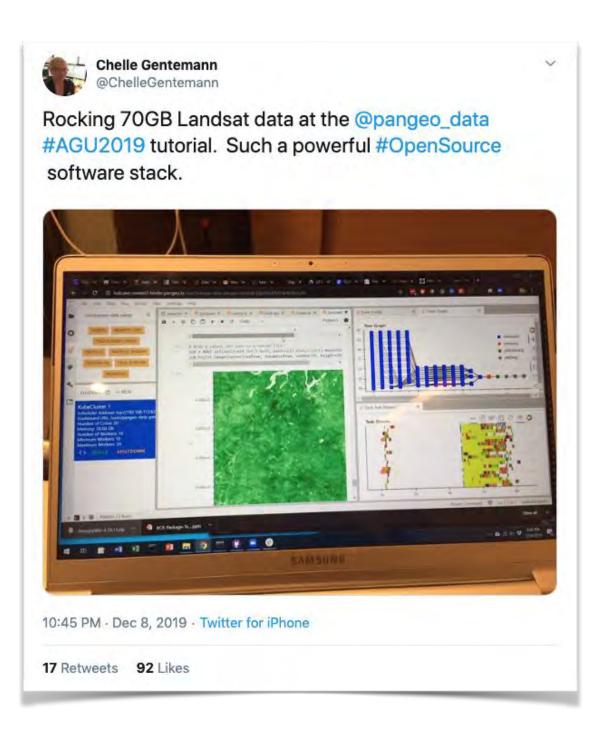


Grass-Roots Solutions















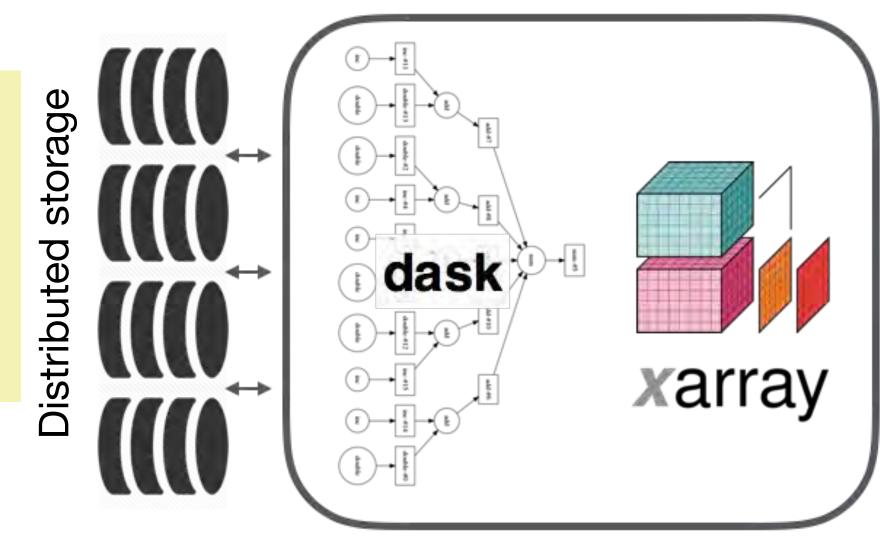




Pangeo Architecture

Cloud / HPC

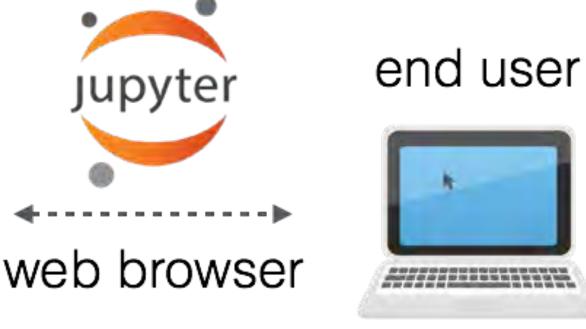
"Analytics Optimized Data Stores" stored on globally-available distributed storage.



Parallel computing system allows users deploy clusters of compute nodes for data processing.

Dask tells the nodes what to do.

Jupyter for interactive data analysis on remote systems



Xarray provides data structures and intuitive interface for interacting with datasets

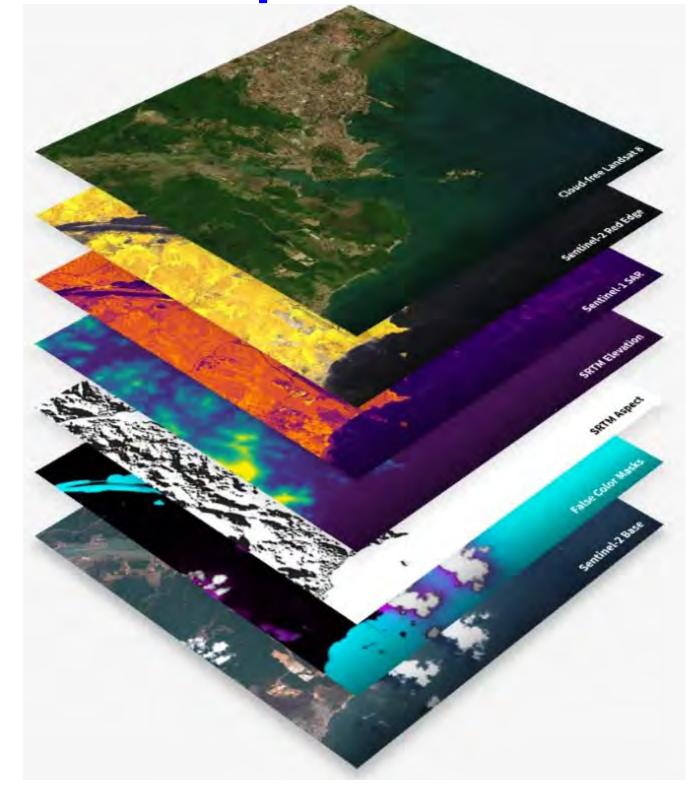




How can data providers reduce barriers?

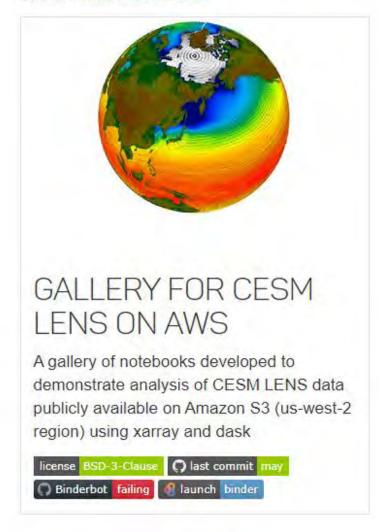
Reimagine how cloud data access and tools can enable transformational science

Publish cloud-optimized data

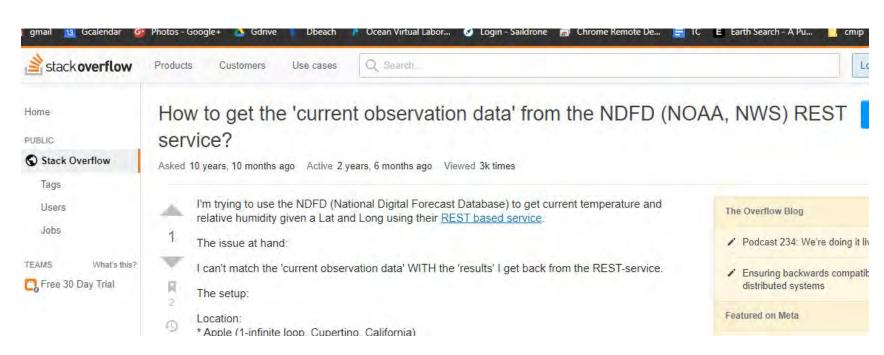


Interactive tutorials PANGEO GALLERY

Welcome to the Pangeo Gallery website. This site containing one or more notebooks. Each gallery is see the Contributor Guide.



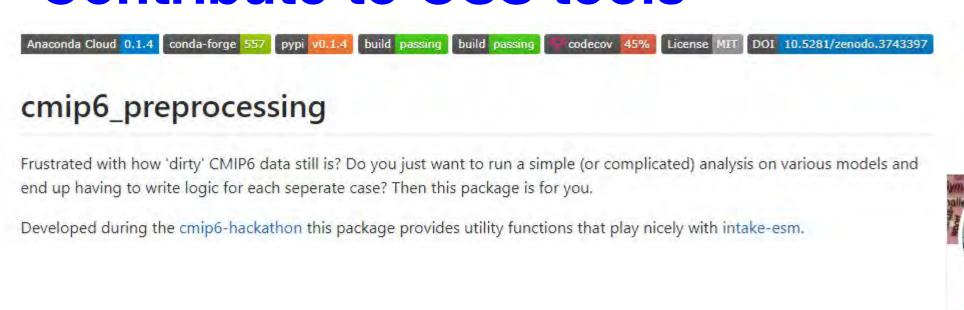
Increase user interactions/feedback



Julius Busecke

@JuliusBusecke Follows you

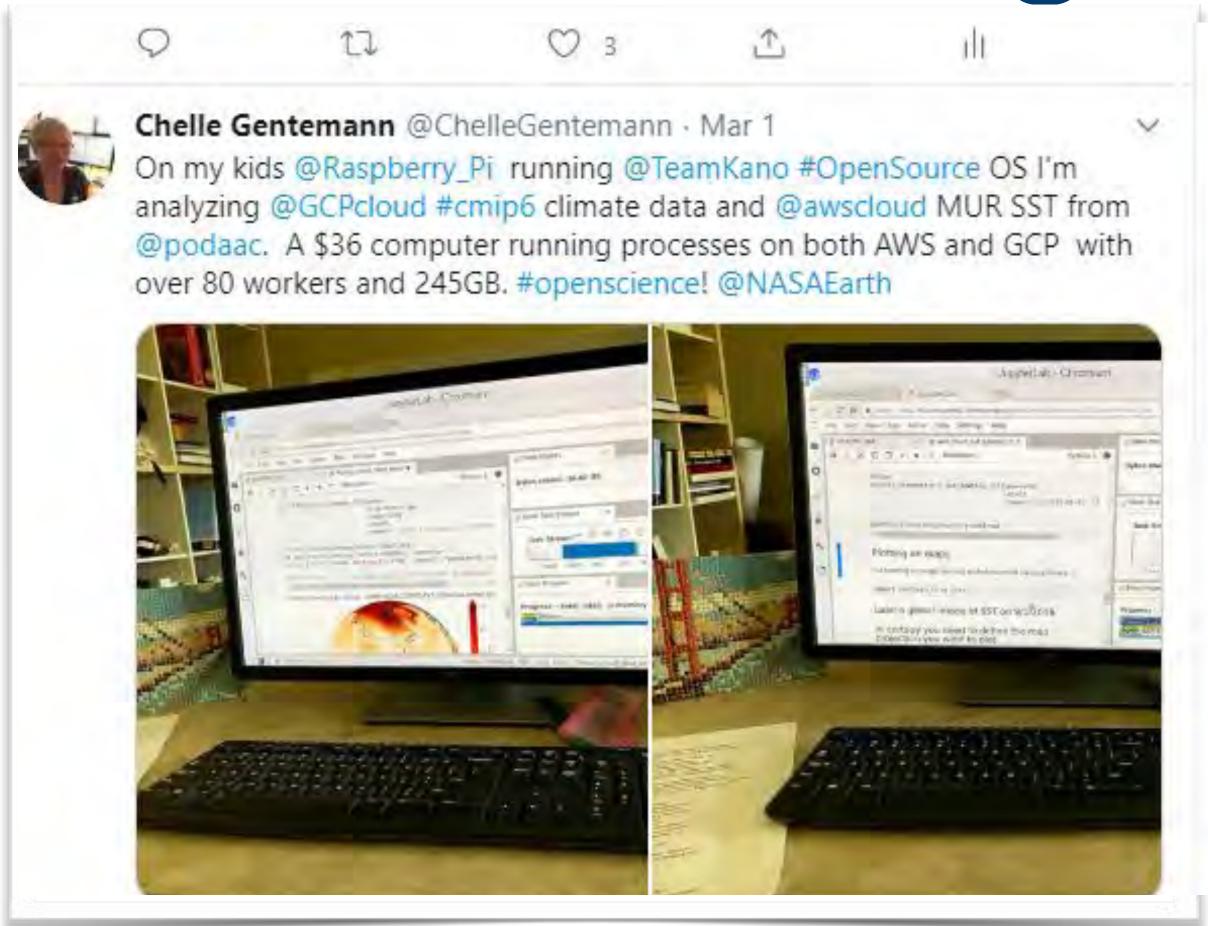
Contribute to OSS tools







How does minimizing barriers to data change science?



Levels the playing field for all who want to contribute





Impacts: Reduce Time to Science

Traditional Project Timeline

80% 10% 10% Data Preparation Batch (download, clean, & organize files) Processing science

Cloud-based Project Timeline

5% 5%
Load Parallel
AODS Processing

90%
Think about science





Impacts: Reproducibility

Reproducibility in data-driven science requires more than just code!

Traditional Project Code

```
# step 1: open data (stored on local hard drive)
>>> data = open_data("/path/to/private/files")
Error: files not found
```

Cloud-based Project Code

```
# step 1: open data (globally accessible)
>>> data = open_data("http://catalog.pangeo.io/path/to/dataset")
# step 2: process data
>>> process(data)
```



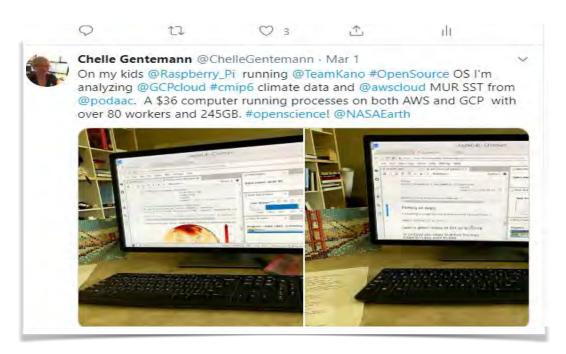


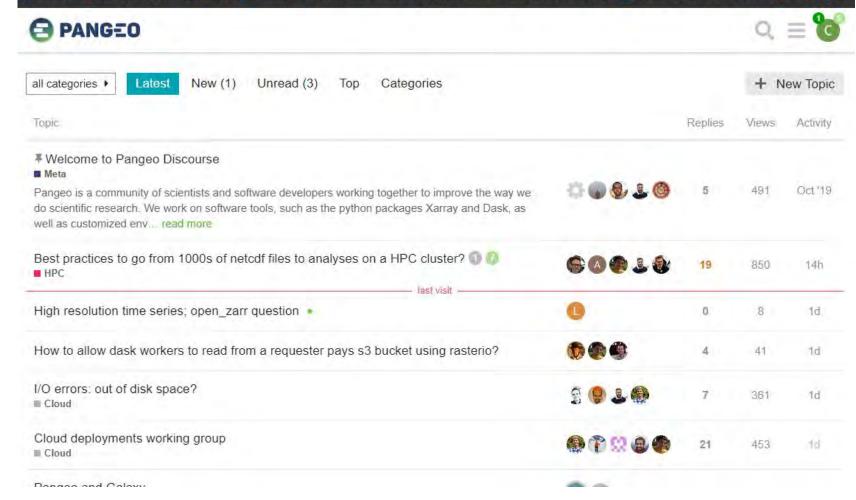
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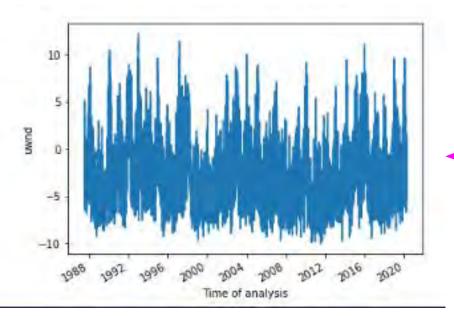




Thank you!







STOP ----- THIS IS DIFFERENT

1 line of code to read in entire 32 year global 25km dataset1 line of code to select a region, calculate & plot a mean time series

in LESS than 1 minute

