Treating gridded geospatial data as point data to simplify analytics

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(3) NASA

Background: NASA GES DISC

Goddard Earth Sciences (GES) Data and Information Services Center (DISC)

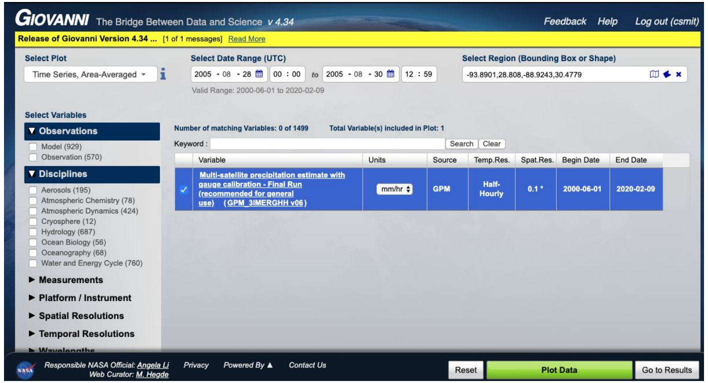
- Archives datasets
  - atmospheric composition
  - water and energy cycles
  - climate variability
- Provides data services

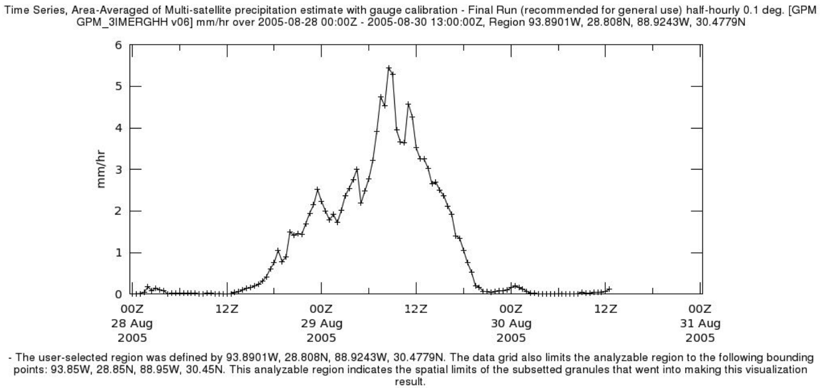
Background: Giovanni

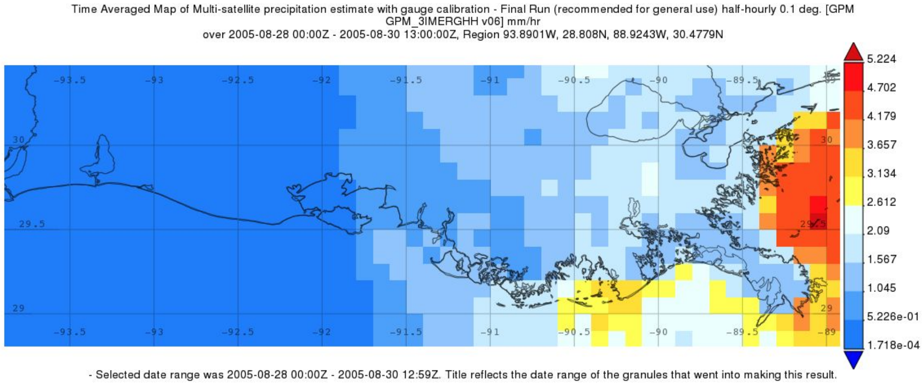
Geospatial Interactive Online Visualization ANd aNalysis Infrastructure (Giovanni)

- Simplify data → science
- Visualizes data in web browser

Background: Giovanni







- 22 summary plots
- > 1000 physical parameters
- > 50 kinds of measurements
- > 20 measurement platforms and instruments

Background: moving to the cloud

On premises

- Technology > 10 years old
- Single server

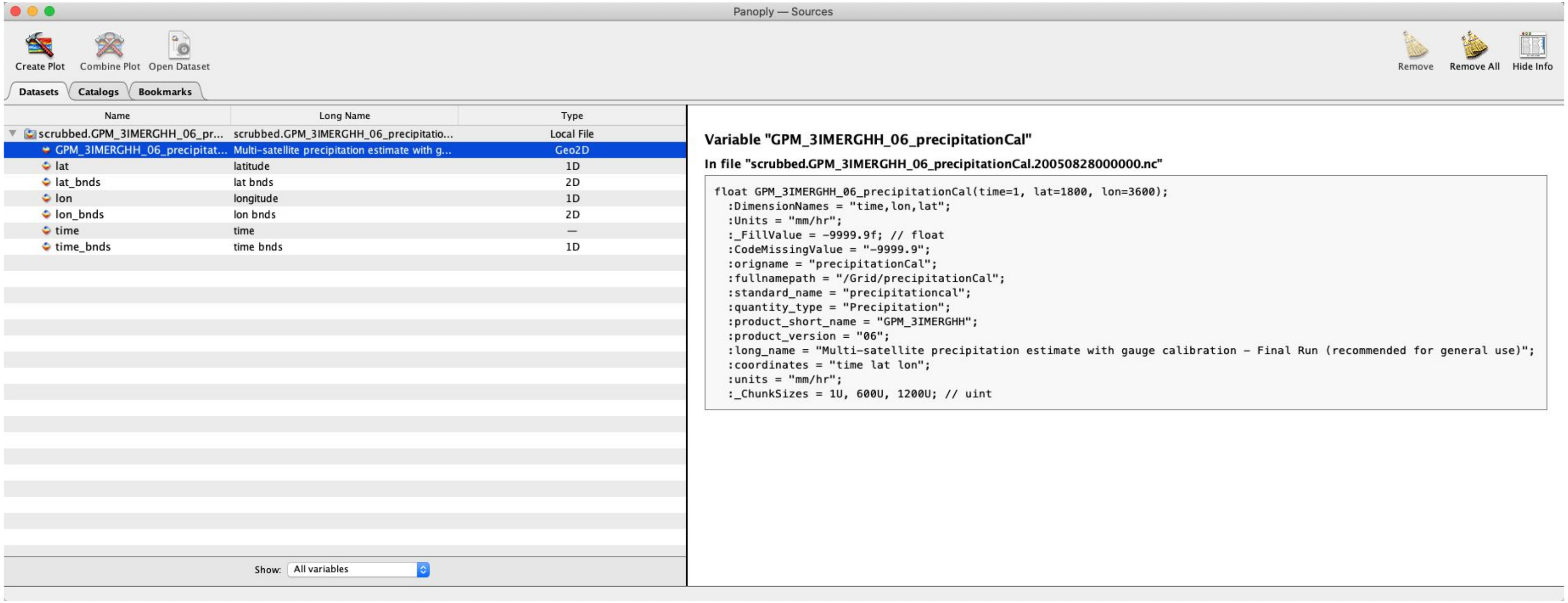
Background: moving to the cloud

Question #1: Data format?

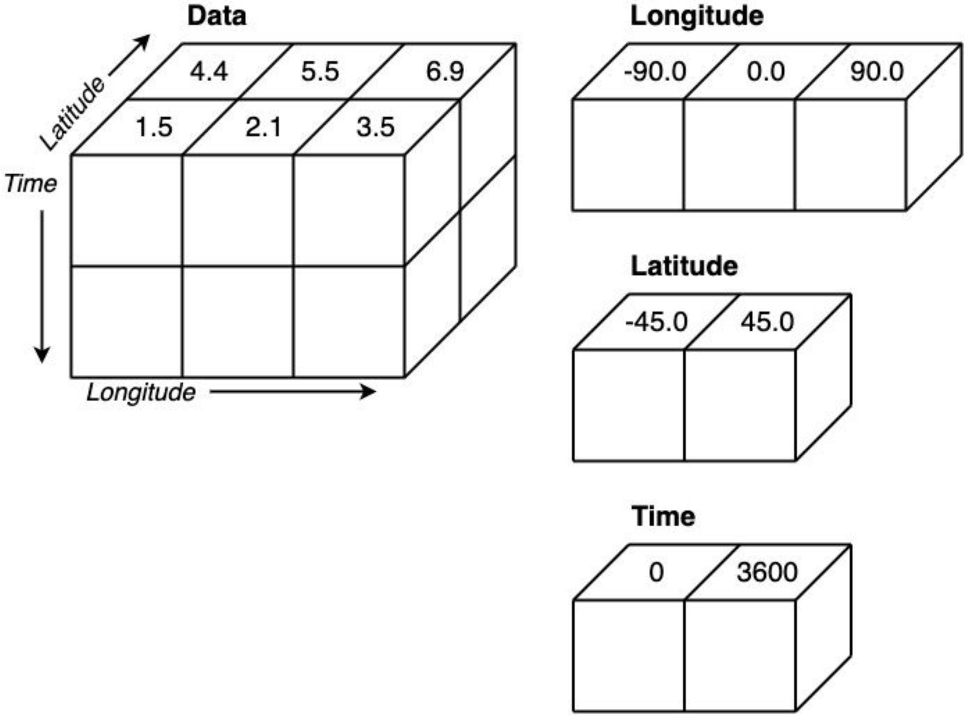
Sidebar: data in the cloud

1. Large datasets → object storage
2. Object storage →
   a. Libraries must support object API.
   b. Data formats must be subsettable in place.

Background: Traditional Data Formats HDF5 and NetCDF4



Background: Traditional Data Formats HDF5 and NetCDF4



Background: HDF5 and NetCDF4

Not (currently) cloud friendly *

- Libraries don't support object storage
- Data can't be subset

* HDF5 has a cloud effort called HSDS, but this requires a data server cluster to be up and running any time you want to access data.

Cloud-friendly data format: Apache Parquet

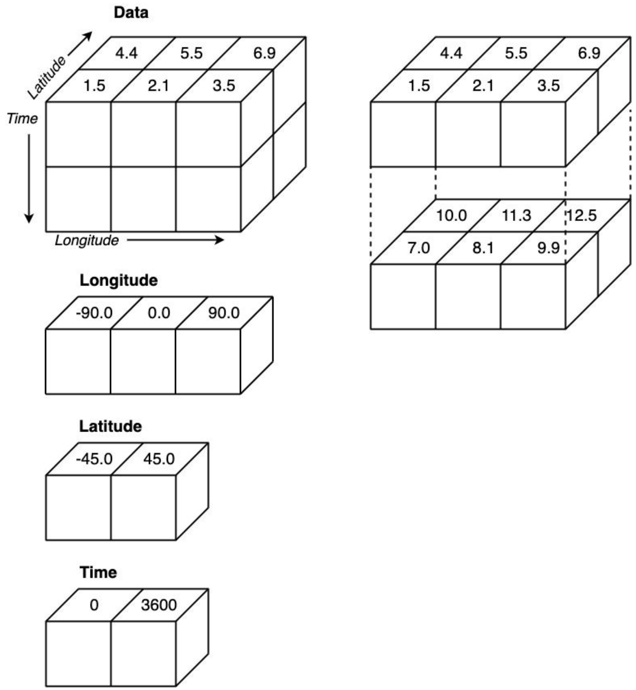
- Columnar data format
- Released 2013
- Part of the Hadoop ecosystem

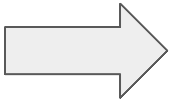
Cloud-friendly data format: Apache Parquet

- Simple data model
- Erases distinctions between different levels and formats of data

Cloud-friendly data format: Apache Parquet

Multi-dimensional array with dimension variables





Point data (Data frame)

Longitude	Latitude	Time	Data
-90.0	-45.0	0	1.5
0.0	-45.0	0	2.1
90.0	-45.0	0	3.5
-90.0	45.0	0	4.4
0.0	45.0	0	5.5
90.0	45.0	0	6.9
-90.0	-45.0	3600	7.0
0.0	-45.0	3600	8.1
90.0	-45.0	3600	9.9
-90.0	45.0	3600	10.0
0.0	45.0	3600	11.3
90.0	45.0	3600	12.5

Example results

Time series with a global average for each day:

- 10.5 years
- Daily, 0.1° data
- ~ 25 billion points

On premises Giovanni:

- ~16500 seconds/4.6 hours
- ~4000 lines of analytics code

Example results: Dask* + Apache Parquet

- **3x faster:** ~4.6 → ~1.4 hours
- **50x less code:** ~4000 → ~75 lines of code

* Dask

- scalable analytics
- cluster or single thread

Dask + Apache Parquet: very simple code

```
def area_average(df,bbox,time_range):
    """
    Builds a dataframe with the area average over the bounding box at each time
    in the time range.

    df: dask dataframe
    bbox: bounding box string in "west,south,east,north" format.
    time_range: time in "YYYY-MM-DDThh:mm:ssZ/YYYY-MM-DDThh:mm:ssZ" format
    """
    # parse the bounding box
    west, south, east, north = [float(v) for v in bbox.split(",")]

    # parse the time range
    start_time, end_time = [string_to_timestamp(s) for s in time_range.split("/")]

    # form the subset and get rid of any NaN values
    subset = df[(df.lat>=south) & \
                (df.lat<=north) & \
                (df.lon>=west) & \
                (df.lon<=east) & \
                (df.time >= start_time) & \
                (df.time<=end_time)].dropna()

    # calculate the cos latitude weight
    subset['weights'] = dask.array.cos(dask.array.multiply(np.pi/180,subset['lat']))

    # multiply the weights by the data values
    subset['weighted_data'] = dask.array.multiply(subset.variable,subset.weights)

    # group by the time, which groups all the data points from the same time together
    grouped = subset.groupby(by="time")

    # calculate the average
    avg = dask.array.divide(grouped.weighted_data.sum(),grouped.weights.sum()).to_frame().reset_index()

    # rename the 'weighted_data' column to 'area average'
    return avg.rename(columns={'weighted_data':'area_average'})
```

Example results: AWS Athena + Apache Parquet (+ 3-dimensional accumulation)

Sidebar: Accumulation to speed up averages

	0	1	2	3	4	5	6	7	8	9
$\vec{X}$	2.3	5.2	8.3	3.0	7.0	1.6	2.2	2.3	6.4	2.3

Sidebar: Accumulation to speed up averages

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$\vec{X}$	2.3	5.2	8.3	3.0	7.0	1.6	2.2	2.3	6.4	2.3

$$avg(5,8) = \frac{1}{4}\sum_{i=5}^{8} x_i$$

Sidebar: Accumulation to speed up averages

$$acc(\vec{X})_i = \sum_{j=0}^{i} x_j$$

Sidebar: Accumulation to speed up averages

	0	1	2	3	4	5	6	7	8	9
$\vec{X}$	2.3	5.2	8.3	3.0	7.0	1.6	2.2	2.3	6.4	2.3
$acc(\vec{X})$	2.3	7.5	15.8	18.8	25.8	27.4	29.6	31.9	38.3	40.6

Sidebar: Accumulation to speed up averages

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$$avg(5,8) = \frac{1}{4}\left(acc(\vec{X})_8 - acc(\vec{X})_4\right)$$

Sidebar: Accumulation to speed up averages

	0	1	2	3	4	5	6	7	8	9
$\vec{X}$	2.3	5.2	8.3	3.0	7.0	1.6	2.2	2.3	6.4	2.3
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$$avg(5,8) = \frac{1}{4}\left(acc(\vec{X})_8 - acc(\vec{X})_4\right)$$

O(1) algorithm!

Sidebar: Accumulation to speed up averages

n-dimension accumulation → 2^n points → still **O(1)** !

Example results: AWS Athena + Apache Parquet (+ 3-dimensional accumulation)

- **3000x faster**: ~4.6 hours → ~5 seconds*
- **10x less code:** ~4000 → ~300 lines of code

* Reported in more detail at the American Geophysical Union (AGU) Fall 2019 Meeting. Abstract: https://agu.confex.com/agu/fm19/meetingapp.cgi/Paper/596820, Poster: https://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/20200000534.pdf

Results

Dash + Apache Parquet

- Code complexity ↓↓↓
- Speed ↑ *(sometimes)*

AWS Athena + Apache Parquet + accumulation

- Code complexity ↓↓
- Speed ↑↑↑

Results

Why not Dask + Apache Parquet + accumulation?

- Poor subsetting*

Why not AWS Athena + Apache Parquet?

- Cost

* Data frame divisions + calculating offsets is fast, but we then can't use main dask API.

Conclusions

- Apache Parquet + high level specification = effortless parallelization
- Data frames = simple code

Looking forward … Zarr?

+ Cloud-native
+ Has multi-dimensional arrays
+ Supports metadata (w/ xarray)

- Library support

Thanks!

NASA GES DISC