Storage growth mitigation through data analysis ready climate datasets using HDF5 Virtual Dataset

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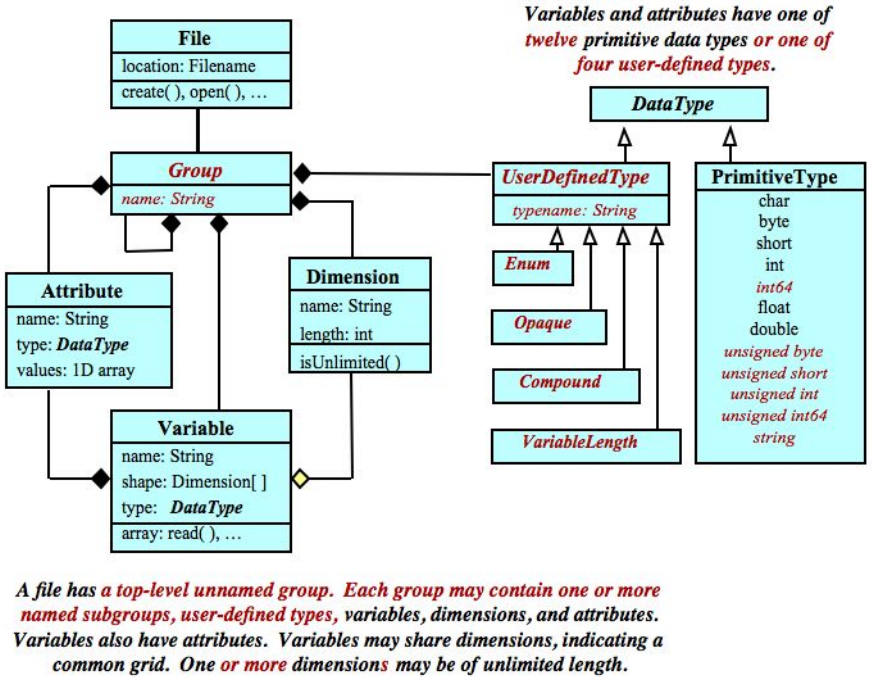
Introduction

- Climate datasets are usually provided in separate files that facilitate dataset management in climate data distribution systems.
  - In ESGF (Earth System Grid Federation) a time series of a variable is split into smaller pieces of data in order to reduce file size.
- This enhances usability for data management in the ESGF distribution system (i.e. file publication and download).
- However, end users need to pre-process and rearrange multiple files as a single data source, in order to obtain a “data analysis ready” dataset, **involving data rewriting and duplication with the corresponding storage growth.**

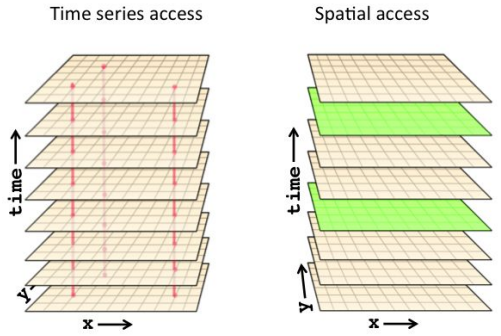
netCDF and HDF5

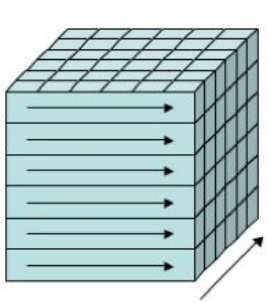
- "netCDF (Network Common Data Form) is a set of software libraries and machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data."
  - Strong commitment for **archival purposes**, libraries with **backward compatibility.**
- Developed by Unidata - https://www.unidata.ucar.edu
- Since version 4 (released in 2008), **netCDF4 files are HDF5** files.
  - It is possible to implement alternative backends.



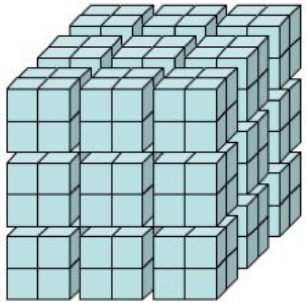
netCDF/HDF5 chunking

- Huge tradeoff between different types of access in a contiguous stored multidimensional array.
- HDF5 files are made of B-trees that store chunks efficiently allowing concurrency, caching and filters.
- Compression and checksum at chunk level.





index order



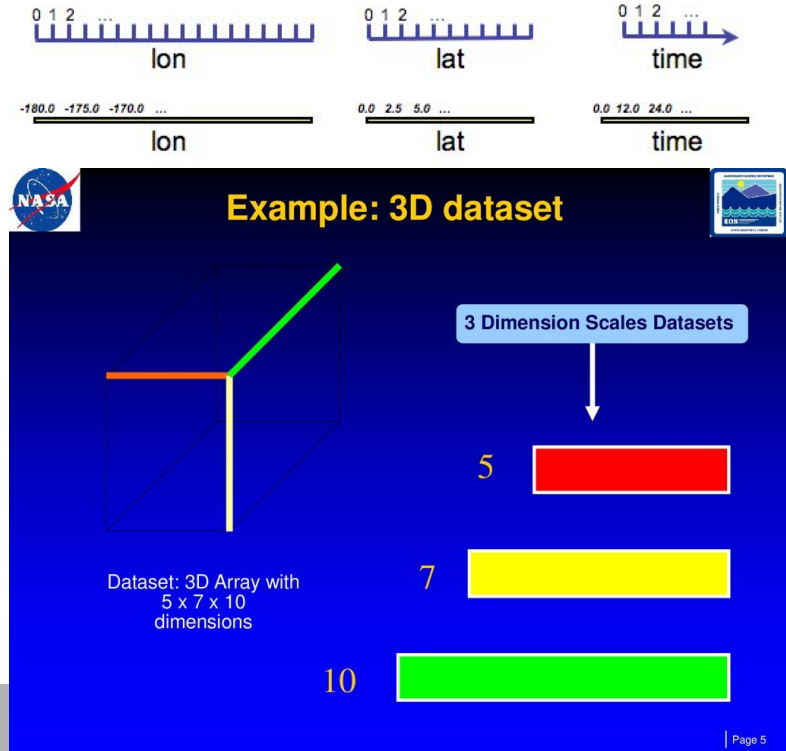
chunked

Storage layout, chunk shapes	Read time series (sec)	Read spatial slice (sec)	Performance bias (slowest / fastest)
Contiguous favoring time range	0.013	180.000	14000.0
Contiguous favoring spatial slice	200.000	0.012	17000.0
Default (all axes equal) chunks, 4673 x 12 x 16	1.400	34.000	24.0
36 KB chunks, 92 x 9 x 11	2.400	1.700	1.4
8 KB chunks, 46 x 6 x 8	1.400	1.100	1.2

From: Unidata Blog

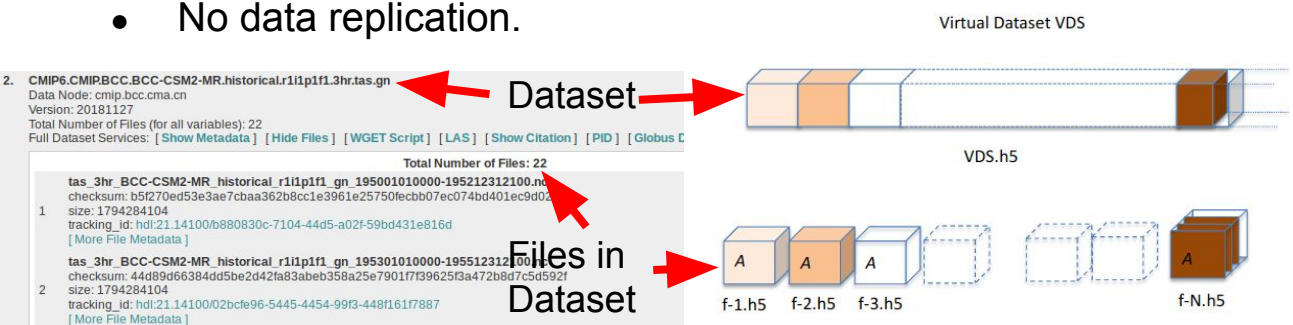
netCDF coordinates / HDF5 dimension scales

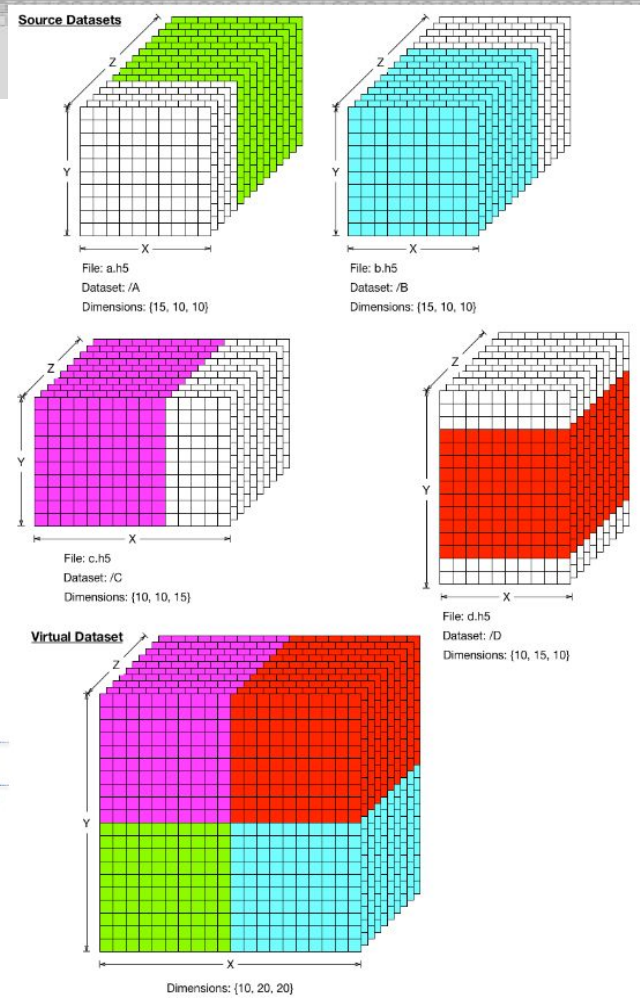
- A variable with the same name as a dimension is called a coordinate variable. To be useful for defining a coordinate system, a coordinate variable:
  - should be one-dimensional.
  - should specify the coordinate value corresponding to each dimension index.
  - should contain no missing values.
  - should have values that are strictly increasing or strictly decreasing.
- In netCDF4, coordinates are implemented using HDF5 dimension scales.
- HDF5 variables (aka datasets) don't use shared dimensions, but define their shape with a dataspace object, which is defined separately for each variable.



HDF5 virtual datasets

- Implemented in the HDF5 library, not in netCDF.
- HDF5 virtual datasets introduce a new dataset storage type that allows a number of multiple HDF5 (and netCDF-4) datasets to be mapped together into a single sliceable dataset via an interface layer.
- Datasets can be mixed in arbitrary combinations, based on range selection mapping to range selection on sources.
- Mapping between different data types. Add, remove or modify existing metadata (i.e. dataset attributes).
- No data replication.



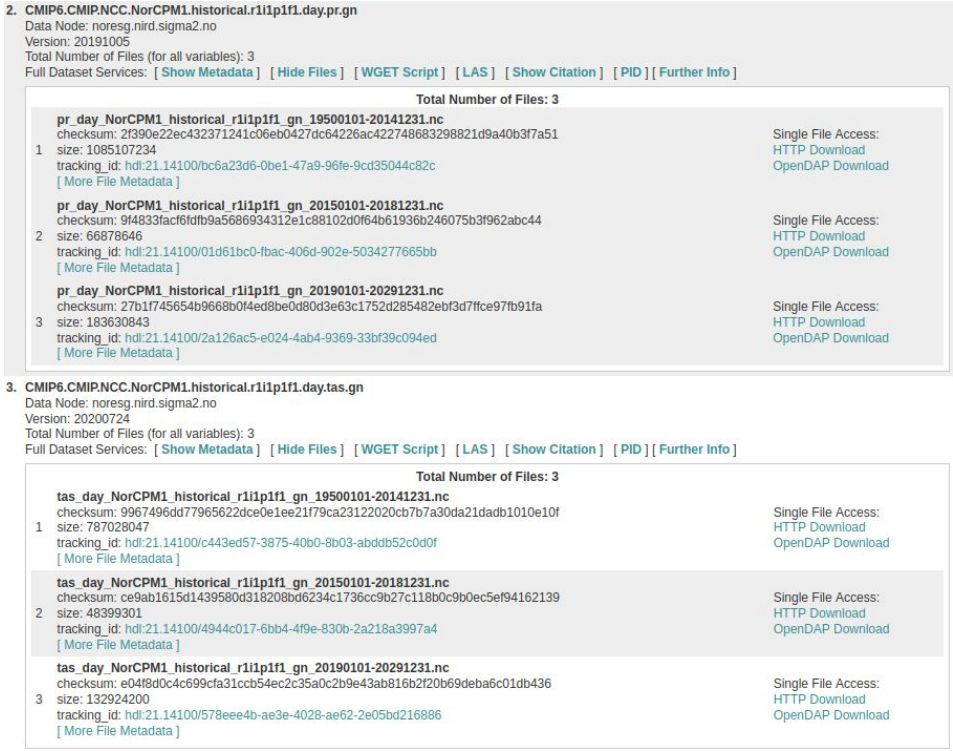


Use case: ESGF virtual datasets

Using **CMIP6 ESGF datasets** as data sources, use HDF5 virtual datasets to generate multiple virtual aggregations following different criteria:

- **Time series aggregation** - Virtual dataset that contains multiple variables with time series joined along the time dimension.
- **Variant label aggregation** - Virtual dataset that spans multiple ESGF datasets (variables and variant labels or ensembles) with time series joined along the time dimension, plus multiple variant labels joined along a new dimension.

Use **netCDF compatible tools** to perform data analysis (xarray, cdo, nco). See the notebook.



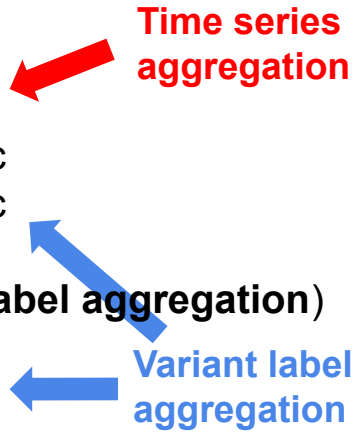
Use case: ESGF virtual datasets

Input files:

- 96x192 lat/lon spatial grid, 240 time steps per file (480 steps for each variable), 2 ensembles

- tas and pr - r1i1p1f1 - 1850-1869 and 1870-1889 (**time series aggregation**)
  - pr_Amon_MPI-ESM1-2-LR_historical_r1i1p1f1_gn_185001-186912.nc
  - pr_Amon_MPI-ESM1-2-LR_historical_r1i1p1f1_gn_187001-188912.nc
  - tas_Amon_MPI-ESM1-2-LR_historical_r1i1p1f1_gn_185001-186912.nc
  - tas_Amon_MPI-ESM1-2-LR_historical_r1i1p1f1_gn_187001-188912.nc

- tas and pr - r2i1p1f1 - 1850-1869 and 1870-1889 (**time series and variant label aggregation**)
  - pr_Amon_MPI-ESM1-2-LR_historical_r2i1p1f1_gn_185001-186912.nc
  - pr_Amon_MPI-ESM1-2-LR_historical_r2i1p1f1_gn_187001-188912.nc
  - tas_Amon_MPI-ESM1-2-LR_historical_r2i1p1f1_gn_185001-186912.nc
  - tas_Amon_MPI-ESM1-2-LR_historical_r2i1p1f1_gn_187001-188912.nc



Examination of the virtual "time series" aggregation dataset

[21]:
```
ds = xarray.open_dataset("timeseries_aggregation.h5")
```

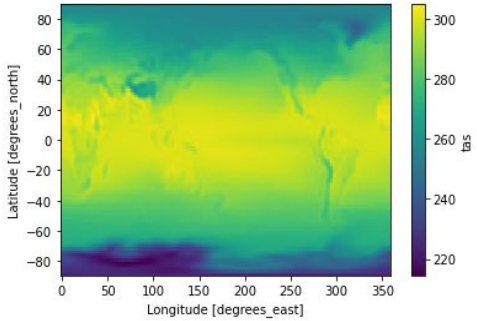
[22]:
```
ds
```

[22]:
```
<xarray.Dataset>
Dimensions:    (bnds: 2, lat: 96, lon: 192, time: 480)
Coordinates:
  * bnds       (bnds) float32 0.0 0.0
  * lat        (lat) float64 -88.57 -86.72 -84.86 -83.0 ... 84.86 86.72 88.57
  * lon        (lon) float64 0.0 1.875 3.75 5.625 ... 352.5 354.4 356.2 358.1
  * time       (time) datetime64[ns] 1850-01-16T12:00:00 ... 1889-12-16T12:00:00
Data variables:
    lat_bnds   (lat, bnds) float64 -89.5 -87.65 -87.65 ... 87.65 87.65 89.5
    lon_bnds   (lon, bnds) float64 -0.9375 0.9375 0.9375 ... 357.2 357.2 359.1
    pr         (time, lat, lon) float32 ...
    tas        (time, lat, lon) float32 ...
    time_bnds  (time, bnds) datetime64[ns] 1850-01-01 1850-02-01 ... 1890-01-01
```

Let's perform a simple plot using xarray.

[23]:
```
ds["tas"].sel(time=slice("18500101", "18691231")).mean(["time"]).plot()
```

[23]:
```
<matplotlib.collections.QuadMesh at 0x7f475cb312e0>
```



Examination of the virtual "variant label" aggregation dataset

[25]:
```
ds = xarray.open_dataset("ensemble_aggregation.h5")
```

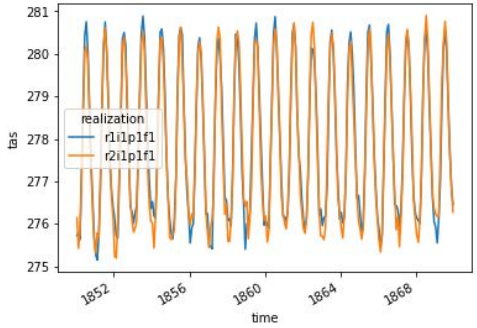
[26]:
```
ds
```

[26]:
```
<xarray.Dataset>
Dimensions:         (bnds: 2, lat: 96, lon: 192, variant_label: 2, time: 480)
Coordinates:
  * bnds            (bnds) float32 0.0 0.0
  * lat             (lat) float64 -88.57 -86.72 -84.86 ... 84.86 86.72 88.57
  * lon             (lon) float64 0.0 1.875 3.75 5.625 ... 354.4 356.2 358.1
  * time            (time) datetime64[ns] 1850-01-16T12:00:00 ... 1889-12-16T1...
  * variant_label   (variant_label) object 'r1i1p1f1' 'r2i1p1f1'
Data variables:
    lat_bnds        (lat, bnds) float64 -89.5 -87.65 -87.65 ... 87.65 87.65 89.5
    lon_bnds        (lon, bnds) float64 -0.9375 0.9375 0.9375 ... 357.2 359.1
    pr              (variant_label, time, lat, lon) float32 ...
    tas             (variant_label, time, lat, lon) float32 ...
    time_bnds       (time, bnds) datetime64[ns] 1850-01-01 ... 1890-01-01
```

Now let's see how easy is to perform multidimensional analysis on climate ready datasets over multiple dimensions. Semantic information about the dimensions is provided by xarray.

[27]:
```
ds["tas"].sel(time=slice("18500101", "18691231")).mean(["lat", "lon"]).plot.line(x="time")
```

[27]:
```
[<matplotlib.lines.Line2D at 0x7f475c9f5ee0>,
 <matplotlib.lines.Line2D at 0x7f475ca20100>]
```



Virtual dataset with NCO

Virtual datasets should be transparent to netCDF clients. However, in practice and due to implementations details, netCDF clients might fail when dealing with HDF5 Virtual Datasets. Here we show how we can use a NCO operator to perform a record average in the variable aggregation virtual dataset.

[30]:
```
!ncra -3 -O timeseries_aggregation.h5 average.nc
```

[31]:
```
!ncdump -hs average.nc
```

```
netcdf average {
dimensions:
        bnds = 2 ;
        lat = 96 ;
        lon = 192 ;
        time = UNLIMITED ; // (1 currently)
variables:
        float bnds(bnds) ;
        double lat(lat) ;
                lat:bounds = "lat_bnds" ;
                lat:units = "degrees_north" ;
                lat:axis = "Y" ;
                lat:long_name = "Latitude" ;
                lat:standard_name = "latitude" ;
        double lat_bnds(lat, bnds) ;
        double lon(lon) ;
                lon:bounds = "lon_bnds" ;
                lon:units = "degrees_east" ;
                lon:axis = "X" ;
                lon:long_name = "Longitude" ;
                lon:standard_name = "longitude" ;
        double lon_bnds(lon, bnds) ;
        float pr(time, lat, lon) ;
                pr:standard_name = "precipitation_flux" ;
                pr:long_name = "Precipitation" ;
                pr:comment = "includes both liquid and solid phases" ;
                pr:units = "kg m-2 s-1" ;
                pr:original_name = "pr" ;
                pr:cell_methods = "area: time: mean" ;
                pr:cell_measures = "area: areacella" ;
                pr:history = "2019-09-11T14:13:17Z altered by CMOR: replaced missing value flag (-9e+33) and corresponding data with standard missing value (1e+20). 2019-09-11T14:13:18Z alt
ered by CMOR: Inverted axis: lat." ;
                pr:missing_value = 1.e+20f ;
        float tas(time, lat, lon) ;
                tas:standard_name = "air_temperature" ;
                tas:long_name = "Near-Surface Air Temperature" ;
                tas:comment = "near-surface (usually, 2 meter) air temperature" ;
                tas:units = "K" ;
                tas:cell_methods = "area: time: mean" ;
```

Conclusions

- HDF5 Virtual Dataset (VDS) is a powerful feature that allows to create compound virtual (data analysis ready) views of existing datasets.
  - **No significant additional storage capacity required.**
- Since netCDF4, netCDF datasets are also HDF5 files. Thus, netCDF applications (xarray, nco, cdo) may also benefit from the VDS feature (netCDF4 required).
- Data analysis ready datasets facilitate and optimize end user data analysis workflows.
- Creation of Virtual Datasets is a form of scientific ETL (Extract, Transform, Load) process.
- netCDF client libraries may find issues when dealing with virtual datasets (e.g. nccopy, due to “storage mode” unknown).
- ESGF based proof of concept available here. High potential for ESGF compute services if used jointly with already available netCDF-java/TDS/OpenDAP services.

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