

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



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This work has been partially supported by:

- PTA program (2016) from Ministerio de Ciencia e Innovación, Spain
- IS-ENES3 – InfraStructure for the European Network for the Earth System Modelling
- INSIGNIA (CGL2016-79210-R) - Contribution to CORDEX Flagship Pilot Studies: regional climate downscaling and data publishing
- CORDyS (PID2020-116595RB-I00) - Contribution to the next generation of CORDEX regional climate projections: Dynamical and Statistical approaches

Project CORDyS (PID2020-116595RB-I00) funded by:



is-enes
INFRASTRUCTURE FOR THE EUROPEAN NETWORK
FOR EARTH SYSTEM MODELLING



co-funded by
FEDER/ERDF
EU funds



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.**

2. CMIP6.CMIPBCC.BCC-CSM2-MR.historical.r1i1p1f1.3hr.tas.gn
 Data Node: cmip.bcc.cma.cn
 Version: 20181127
 Total Number of Files (for all variables): 22
 Full Dataset Services: [[Show Metadata](#)] [[Hide Files](#)] [[WGET Script](#)] [[LAS](#)] [[Show Citation](#)] [[PID](#)] [[Globus Download](#)]

Total Number of Files: 22

1 tas_3hr_BCC-CSM2-MR_historical_r1i1p1f1_gn_195001010000-195212312100.nc
 checksum: b5f270ed53e3ae7cbaa362b8cc1e3961e25750fecbb07ec074bd401ec9d02748
 size: 1794284104
 tracking_id: hdi:21.14100/b880830c-7104-44d5-a02f-59bd431e816d
[\[More File Metadata \]](#)

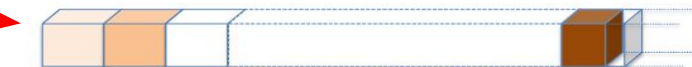
2 tas_3hr_BCC-CSM2-MR_historical_r1i1p1f1_gn_195301010000-195512312100.nc
 checksum: 44d89d66384dd5be2d42fa83abeb358a25e7901f7f39625f3a472b8d7c5d592f
 size: 1794284104
 tracking_id: hdi:21.14100/02bcfe96-5445-4454-99f3-448f161f7887
[\[More File Metadata \]](#)

Dataset

Files in Dataset

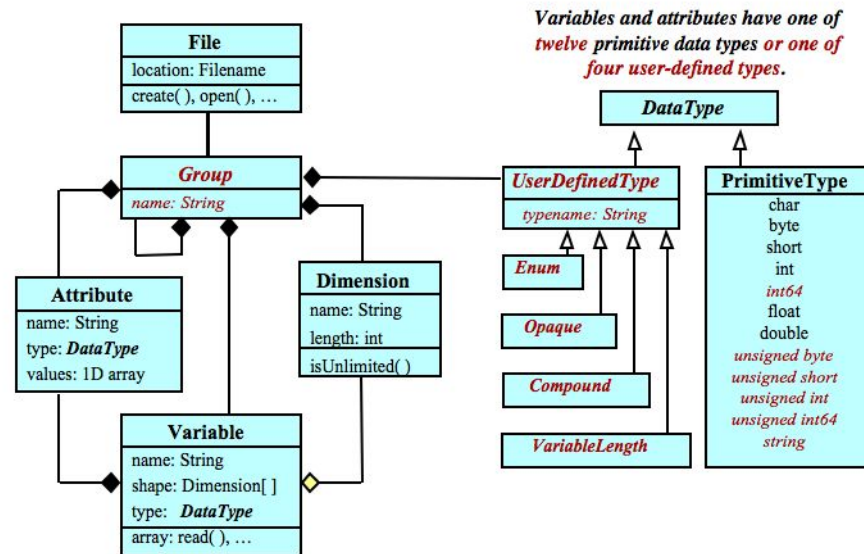
Virtual Dataset VDS

VDS.h5



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.

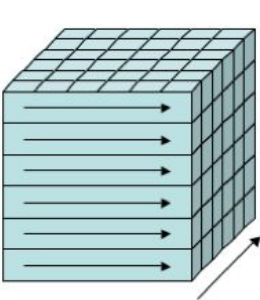


Variables and attributes have one of twelve primitive data types or one of four user-defined types.

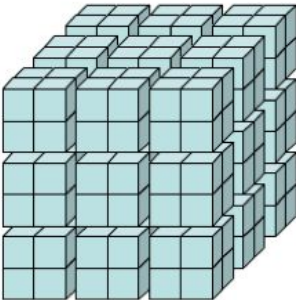
A file has a top-level unnamed group. Each group may contain one or more named subgroups, user-defined types, variables, dimensions, and attributes. Variables also have attributes. Variables may share dimensions, indicating a common grid. One or more dimensions may be of unlimited length.

netCDF/HDF5 chunking

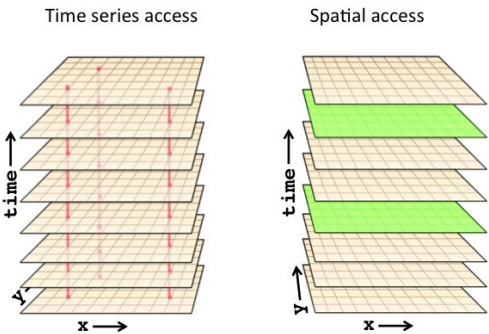
- Huge tradeoff between different types of access in a contiguous stored multidimensional array.
- HDF5 files are made of B-trees that store chunks efficiently allowing concurrency, caching and filters.
- Compression and checksum at chunk level.



index order



chunked

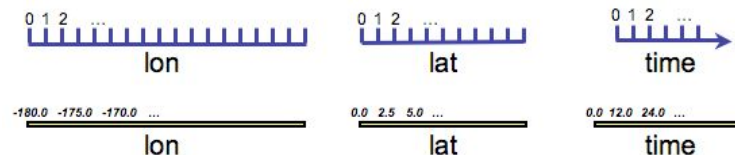


Storage layout, chunk shapes	Read time series (sec)	Read spatial slice (sec)	Performance bias (slowest / fastest)
Contiguous favoring time range	0.013	180.000	14000.0
Contiguous favoring spatial slice	200.000	0.012	17000.0
Default (all axes equal) chunks, 4673 x 12 x 16	1.400	34.000	24.0
36 KB chunks, 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

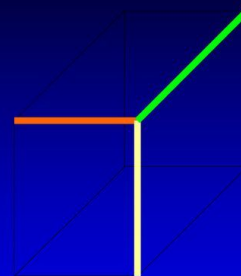
From: [Unidata Blog](#)

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.



Example: 3D dataset



Dataset: 3D Array with
5 x 7 x 10
dimensions

3 Dimension Scales Datasets

5



7

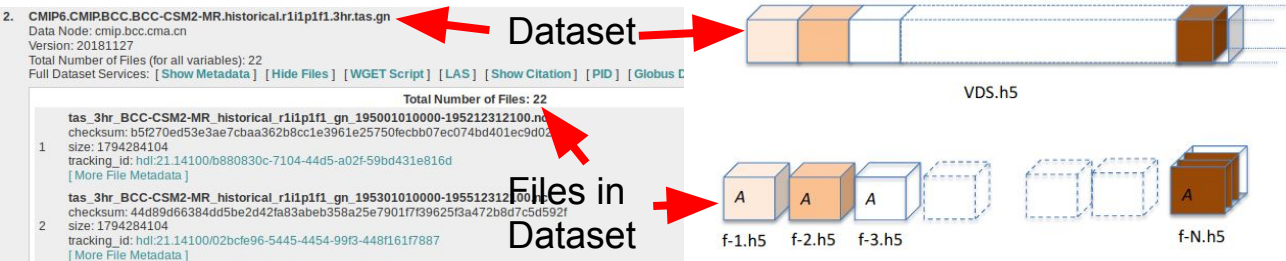
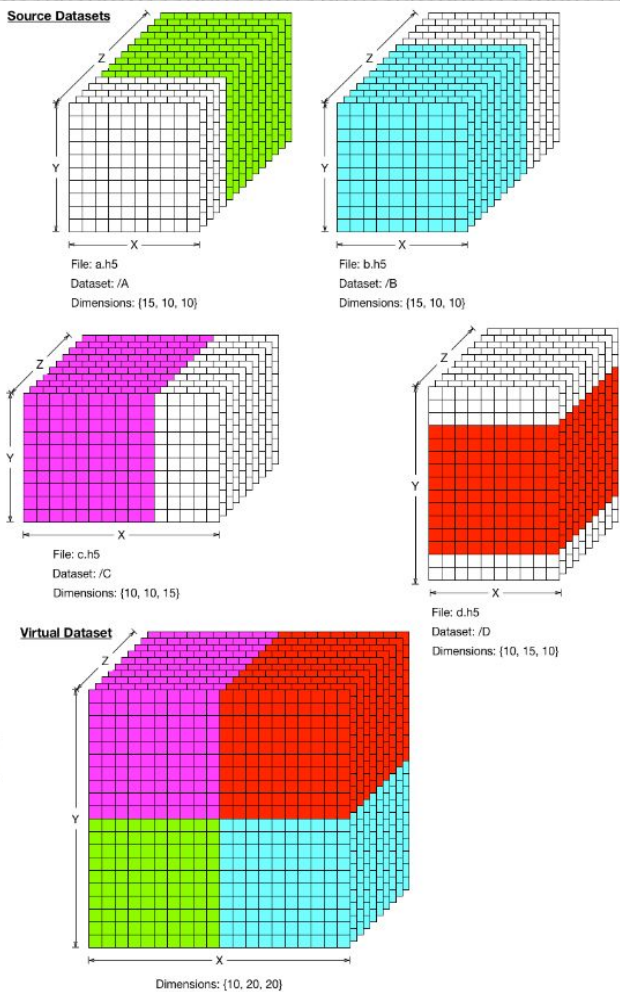


10



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.



2. CMIP6.CMIPBCC.BCC-CSM2-MR.historical.r11p1f1.3hr.tas.gn
Data Node: cmip.bcc.cma.cn
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Total Number of Files: 22

tas_3hr_BCC-CSM2-MR_historical_r11p1f1_gn_195001010000-19512312100.nc
checksum: b5f270ed5e3ae7cbba362b8cc1e3961e25750fecb07ec074bd401ec9d02
size: 1794284104
tracking_id: hdl:21.14100/b880830c-7104-44d5-a02f-59bd431e816d
[[More File Metadata](#)]

tas_3hr_BCC-CSM2-MR_historical_r11p1f1_gn_195301010000-195512312100.nc
checksum: 44d89d66384dd5be2d42fa83abeb358a25e7901f7f39625f3a472b8d7c5d592f
size: 1794284104
tracking_id: hdl:21.14100/02bcfe96-5445-4454-99f3-448f161f7887
[[More File Metadata](#)]

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](#).

2. CMIP6.CMIP.NCC.NorCPM1.historical.r1i1p1f1.day.pr.gn

Data Node: noresg.nird.sigma2.no
Version: 20191005
Total Number of Files (for all variables): 3
Full Dataset Services: [Show Metadata] [Hide Files] [WGET Script] [LAS] [Show Citation] [PID] [Further Info]

Total Number of Files: 3

pr_day_NorCPM1_historical_r1i1p1f1_gn_19500101-20141231.nc

checksum: 2f390e22ec432371241c06eb0427dc64226ac422748683298821d9a40b37a51
size: 1085107234
tracking_id: hdi:21.14100/bc6a23d6-0be1-47a9-96fe-9cd35044c82c
[More File Metadata]

Single File Access:
[HTTP Download](#)
[OpenDAP Download](#)

pr_day_NorCPM1_historical_r1i1p1f1_gn_20150101-20181231.nc

checksum: 9f4833f6c6fdb9a5686934312e1c88102d0f64b61936b246075b3f962abc44
size: 66878646
tracking_id: hdi:21.14100/01d61bc0-fbac-406d-902e-5034277665bb
[More File Metadata]

Single File Access:
[HTTP Download](#)
[OpenDAP Download](#)

pr_day_NorCPM1_historical_r1i1p1f1_gn_20190101-20291231.nc

checksum: 27b1f745654b9668b0f4ed8be0d80d3e63c1752d285482ebf3d7f97b91fa
size: 183630843
tracking_id: hdi:21.14100/2a126ac5-e024-4ab4-9369-33bf39c094ed
[More File Metadata]

Single File Access:
[HTTP Download](#)
[OpenDAP Download](#)

3. CMIP6.CMIP.NCC.NorCPM1.historical.r1i1p1f1.day.tas.gn

Data Node: noresg.nird.sigma2.no
Version: 20200724
Total Number of Files (for all variables): 3
Full Dataset Services: [Show Metadata] [Hide Files] [WGET Script] [LAS] [Show Citation] [PID] [Further Info]

Total Number of Files: 3

tas_day_NorCPM1_historical_r1i1p1f1_gn_19500101-20141231.nc

checksum: 9967496dd77965622dce0e1ee21f79ca23122020cb7b7a30da21dad1010e10f
size: 787028047
tracking_id: hdi:21.14100/c443ed57-3875-40b0-8b03-abddb52c0d0f
[More File Metadata]

Single File Access:
[HTTP Download](#)
[OpenDAP Download](#)

tas_day_NorCPM1_historical_r1i1p1f1_gn_20150101-20181231.nc

checksum: ce9ab1615d1439580d318208bd6234c1736cc9b27c118b0c9b0ec5ef94162139
size: 48399301
tracking_id: hdi:21.14100/4944c017-6bb4-4f9e-830b-2a218a3997a4
[More File Metadata]

Single File Access:
[HTTP Download](#)
[OpenDAP Download](#)

tas_day_NorCPM1_historical_r1i1p1f1_gn_20190101-20291231.nc

checksum: e048d0c4c699cfa31ccb54ec2c35a0c2b9e43ab816b2f20b69deba6c01db436
size: 132924200
tracking_id: hdi:21.14100/578ee4b-ae3e-4028-ae62-2e05bd216886
[More File Metadata]

Single File Access:
[HTTP Download](#)
[OpenDAP Download](#)

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



Time series aggregation



Variant label aggregation

Santander Meteorology Group

Examination of the virtual "time series" aggregation dataset

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

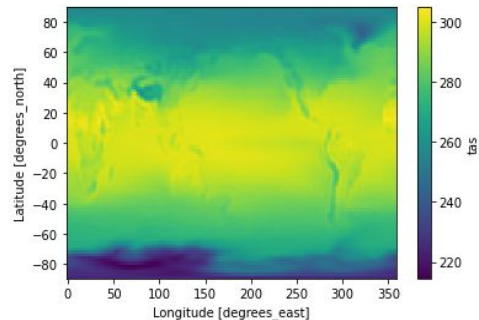
[22]: ds

[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")

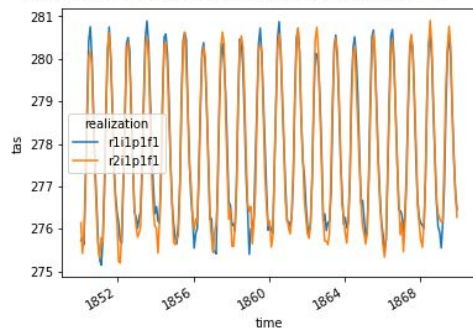
[26]: ds

[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 'r1ilp1f1' 'r2ilp1f1'
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 -0 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 altered 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.

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



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