Data Management: Data Standardization

Angelika Heil Martin Schupfner Fabian Wachsmann

Data Management: Data Standardization by Heil, A; Schupfner, M; Wachsmann, F. . Slides presented at the DKRZ User Workshop, 13. October 2022, Hamburg. This work is licensed under <u>CC BY 4.0</u>.





Agenda Data Standardization Workshop: October 13, 2022

11:45 – 12:05	Overview: CF conventions, NetCDF formats, FAIR data publication, CMORization, Quality Assurance	Angelika Martin
12:05 – 12:25	Exercise: Simple data standardization	Angelika
12:25 – 13:00	Exercise: CMORization	Martin
13:00 - 14:00	Lunch Break	

We prepared various Jupyter notebooks for this training... see our Jupyter book at https://dkrz-user-workshop-dm-training1.gitlab-pages.dkrz.de/data-standardization/intro.html or our gitlab repository https://gitlab.dkrz.de/dkrz-user-workshop-dm-training1/data-standardization

Please try them out on DKRZ's JupyterHub: https://jupyterhub.dkrz.de/



Find the instructions also here (to copy paste commands if necessary): https://dkrz-user-workshop-dm-training1.gitlab-pages.dkrz.de/data-standardization/intro.html First, visit https://jupyterhub.dkrz.de and click on Preset start C+ Logout Home Token Services-Levante Documentation b309100 DKRZ DEUTSCHE **KLIMARECHENZENTRUN Spawner Options**





Select the job profile from below and enter one of your accounts that allows you to launch parallel jobs on levante. Reservation and QoS can be left empty. Then click on Start.

Server Options

Reset options

Select	a	job	profile:	
--------	---	-----	----------	--

· · · · ·	
20 GB memory, interactive, 12:00h	
Account (account):	If you do not know any of your accounts:
bk1261	 Open a terminal ssh-login to levante
Reservation (reservation):	 Ssiriogin to levalue Execute the <i>groups</i> command to list all projects, and try one of the 6-digit group names
QoS (qos): Start	~\$ ssh -X b309100@levante.dkrz.de [b309100@levante5 ~]\$ groups id0853 b b309 bk1261

Now wait until your server is starting up...you will be redirected automatically to the JupyterLab Interface

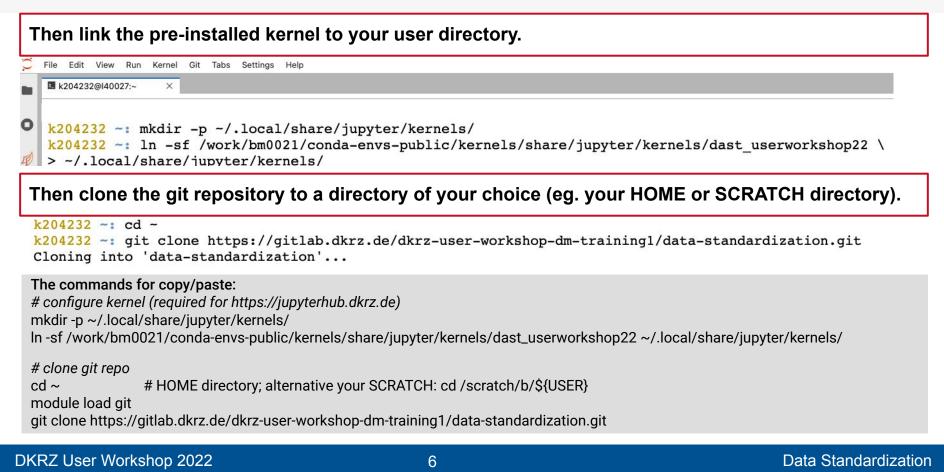


To be able to use the pre-installed jupyter kernel, open a terminal with jupyterhub.

\bigcirc	File Edit View Run Kerne	el Git Tabs	Settings Help	
	New New Launcher	, ራ # L	Console	
0	Open from Path		 Terminal E Text File 	
围	New View for New Console for Activity		Markdown File R R File	Notebook
٠	Close Tab Close and Shutdown Close All Tabs	て W へ ☆ Q	Python FileJulia File	

Alternative: open a terminal on your local machine and ssh-login to levante ...

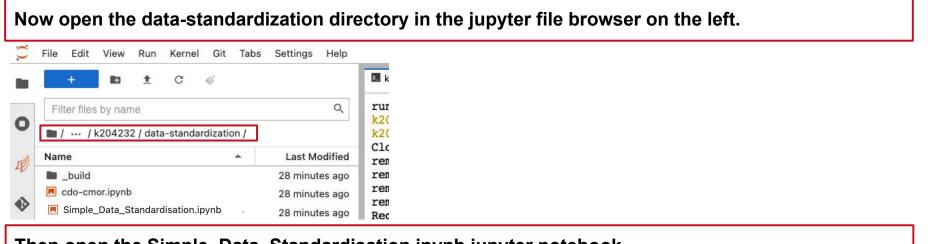






Data Standardization

Set up jupyterhub



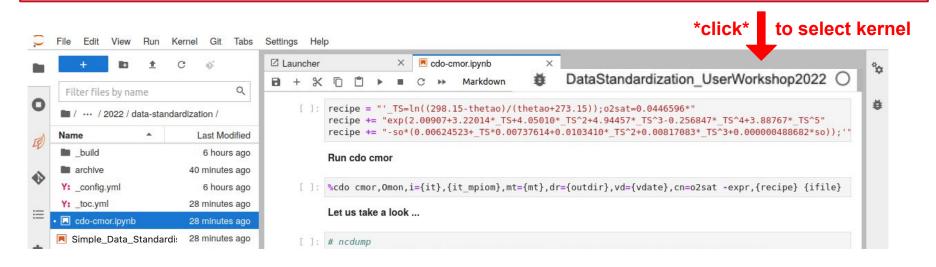
Then open the Simple_Data_Standardisation.ipynb jupyter notebook.

()	File	Edit	View	Run	Ker	nel	Git	Tabs	Set	tings	Help																								
		+		±	C	<	ş						k204								_User_				8.0										
0	Fi	lter files	s by na	me							Q		a) +	ж	D		•		C •	•	Markd	own 🗸	ŧ	C	git			0	Da	taStanda	ardiza	tion_U	serWor	kshop2	.022 ()
U		/ /	k20423	32 / dat	a-star	dard	izatio	n /																											
围	Nar	174 12/2010						•		1.1.2.1.10	odified	-																							
		_build _config	g.yml								tes ago tes ago																				<	-			KRZ
		Simpl	le_Data	a_Stan	dardi	satio	n.ipyı	nb	39	minut	tes ago	L			De	em	0.	Jup	yte	er	No	teb	00	k f	or t	the DK	(RZ Us	ser W	/orl	csho	р		KLI		DEUTSCHES

DKRZ User Workshop 2022



When you open any of the workshop notebooks (*.ipynb files) in the data-standardization folder, please check that the fitting kernel "DataStandardization_UserWorkshop22" is selected





Why Do We Need Data Standardization?

Data standardization means, e.g. to rewrite data

- in a common file format (e.g. netCDF)
- with similar data structures
- with sufficient & consistent metadata

Data standardization

- is vital when you want to reuse your data on the longer term
- is vital when sharing data with others
- accelerates scientific progress, particularly in the era of Big Data



Why Do We Need Data Standardization?

Data standardization means, e.g., to rewrite data....

- in a common file format (e.g. netCDF)
- with similar data structures
- with sufficient & consistent metadata

Data standardization

- is vital when you want to reuse your data on the longer term
- is vital when sharing data with others
- accelerates scientific progress, particularly in the era of Big Data
- is a precondition for a successful data publication

Announcement: FAIR data in Earth science nature



nature.ttpm//www.nature.com/articles/d41586-019-00075-3 Announcement: FAIR data in Earth science Nature - Nature backs the Enabling FAIR Data initiative and requires authors to deposit data in community repositories.







Data Standardization – Make Your Data FAIR!

The FAIR principles* are the most widely adopted guiding principles for scientific data management.

Data are described by rich, **meaningful metadata**. Data and metadata are assigned unique **persistent identifiers** (PIDs). Data and metadata are indexed in a searchable Data Catalogue.

Data and metadata can be **accessed** through **standard data protocols**. Metadata remain accessible even if the data are no longer available.

Data are readable for machines.

Metadata are defined in **controlled vocabularies** (**CVs**; "standardised terms"). Metadata include cross-references to related metadata (meaningful links).

Data are clearly described and contain detailed **provenance** information. Data are released with a clear **data licensing** status. Data and metadata meet relevant **domain standards** (e.g. file formats).

Findable

Accessible

Interoperable

Reusable

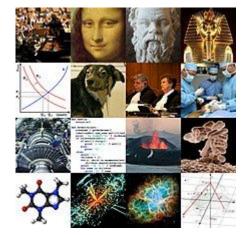


Why Do We Need Data Standardization?

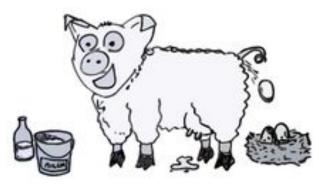
No Data Standard



Discipline/Projectspecific Standard



One Standard for All Data



Data Standardization Scale

HOW STANDARDS PROLIFERATE: (SEE: A/C CHARGERS, CHARACTER ENCODINGS, IN STANT MESSAGING, ETC.)

SITUATION: THERE ARE 14 COMPETING STANDARDS.

14?! RIDICULOUS! WE NEED TO DEVELOP ONE UNIVERSAL STANDARD THAT COVERS EVERYONE'S USE CASES. YEAH!



SITUATION: THERE ARE 15 COMPETING STANDARDS.



(Meta)data Standards in Earth System Sciences (ESS)

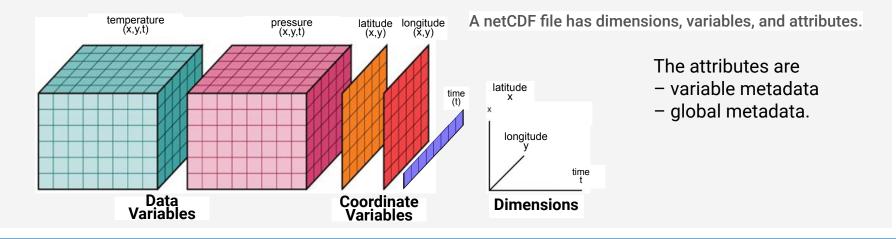
- Data Formats
 - netCDF(3,4), HDF5, GeoTIFF, GRIB...(self-describing) Ο
- General (Meta)data
 - CF (Climate and Forecast) metadata conventions Ο CF standard names: controlled vocabulary (CV)
 - COARDS conventions (predecessor of CF) \bigcirc
- Discipline/Project-Specific (Meta)data
 CMIP5/6
 ESA CCI; Copernicus; ATMODAT;...

building upon CF



Climate and Forecast (CF) Metadata Conventions

- most widely used community standard in ESS for encoding data in netCDF data format ("CF-netCDF").
- CF provides guidance on how to provide a definitive description of what the data in each variable represents, the spatial and temporal properties of the data, and the placement of metadata within the netCDF file.



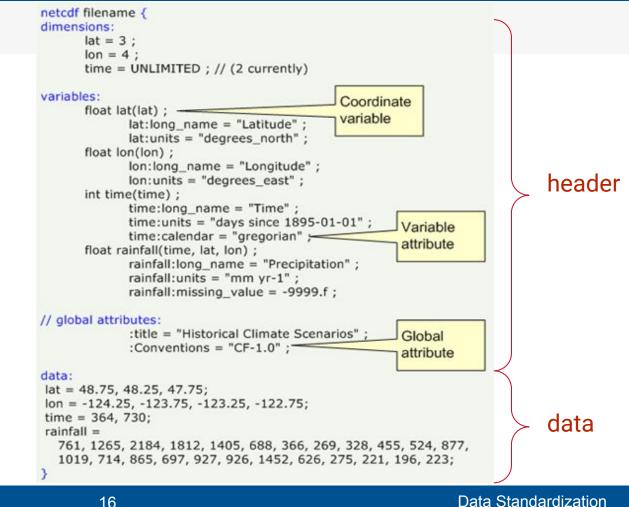


The netCDF Header

ncdump -h filename

- Dimensions 1)
- 2) Variables incl. Variable Attributes
- 3) Global attributes

Data 4





CF Standard Names

- are a controlled vocabulary (CV)
 CF standard name ≠ netCDF variable name
- used to label the geophysical variables within CF compliant data
- have a precise definition and an prescribed "canonical" units (=> Udunits2)

http://cfconventions.org/Data/cf-standard-names/current/build/cf-standard-name-table.html

Standard Name	Canonical Units				
<pre>vair_temperature</pre>					
Air temperature is the bulk temperature of the air, not the surface (skin) temperature.	IX				

What are canonical units?

Every CF standard name must be specified together its canonical units, except for unitless quantities. Instead of the canonical units, any Udunits2-compatible units can be specified. Udunits-2 is the Unidata units library <u>https://github.com/Unidata/UDUNITS-2</u>

DKRZ User Workshop 2022 New CF standard names can be proposed to the CF community! Data Standardization



CF Standard Names

- are a controlled vocabulary (CV)
- used to label the geophysical variables within CF compliant data
- have a precise definition and an prescribed "canonical" unit (=> Udunits2)
- are used as value for the **standard_name** variable attribute, e.g.

```
float tas(time, rlat, rlon);

tas:standard_name = "air_temperature";

tas:units = "K";

tas:coordinates = "lon lat height";

tas:long_name = "Near-Surface Air Temperature";
```



Software that "understands" CF-netCDF

python tools implementing an abstracted "CF data model"

- *cfdm* and the extensions *cf-python* and *cdf-plot/cf-view*
- iris

tools that support parts of the CF conventions

- CDO, NCO
- xarray, cf-xarray



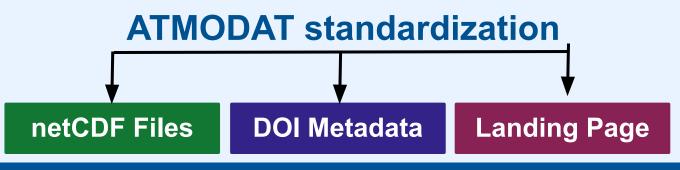
ATMODAT standard for simple FAIR data publications

Ganske et al. (2021) https://doi.org/10.35095/WDCC/atmodat_standard_en_v3_0

- CF-netCDF data files
- a set of **mandatory**, **recommended** and **optional metadata**
- atmodat checker can check compliance
- assumes a open license **data publication** with a **DataCite DOI**
- highlighted in WDCC with

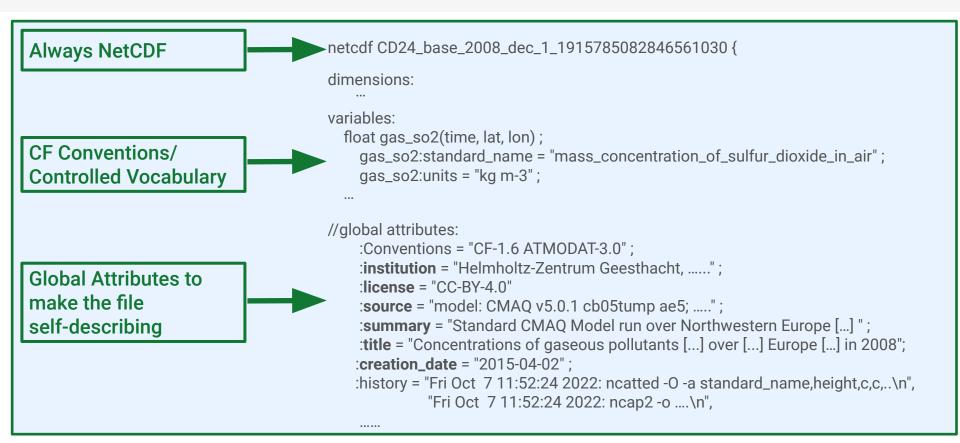


a new quality seal for FAIR & open Earth System Science data





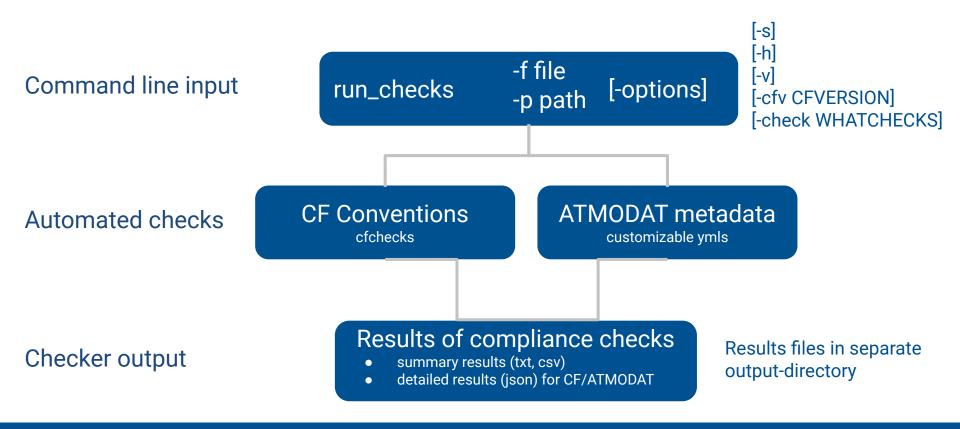
Requirements for the netCDF files





atmodat checker

https://github.com/AtMoDat/atmodat_data_checker





atmodat checker

https://github.com/AtMoDat/atmodat_data_checker

create summary

Example short summary.txt: run_checks.py -s -p myfolder/

Short summary of checks:

Checking against: atmodat_standard:3.0, CF table version: 77 Version of the AtMoDat checker: 1.1.0 Checked at: 2021-08-11T14:54:17.517485

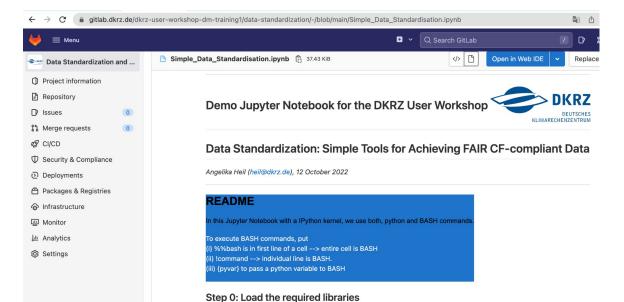
Number of checked files: 3 Total checks passed: 4/31 Mandatory checks passed: 2/4 Recommended checks passed: 2/18 Optional checks passed: 0/9 CF checker errors: 1



Please try it out!

https://gitlab.dkrz.de/dkrz-user-workshop-dm-training1/data-standardization

Jupyter Notebook: Simple_Data_Standardisation.ipynb



DKRZ User Workshop 2022

Data Standardization



Project specific data standardization - CV & DRS

Project specific standardization - Example CMIP6

 \rightarrow The CMIP6 metadata requirements build on CF

CMIP6 Data Reference Syntax (DRS) and Controlled Vocabularies (CVs) prescribe

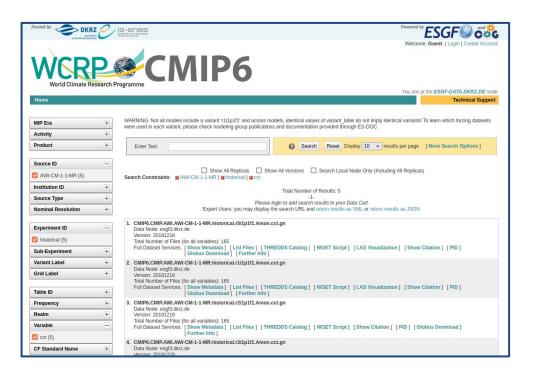
- global attributes related to
 - experiment
 - variant / simulation
 - institution
 - licensing restrictions
 - etc
- components to compose filenames and directory structure
 - \rightarrow These components uniquely define each dataset (i.e. a single variable of a single simulation)
- variables and related attributes ("MIP tables" / "CMOR tables")



Project specific data standardization - CV & DRS

DRS/CV characterize the data and are essential for organizing, managing and accessing large data collections by

- enabling the intercomparison of data from different sources
- helping to define and structure data catalogs (eg. intake catalogs)
- serving as search facets in data portals (eg. <u>ESGF</u> Data Portal)





Project specific data standardization - CMOR

<u>CMOR</u> - Climate Model Output Rewriter

- library with functions to read, reformat and write climate data variables
- reads the official project standard configuration
 → no user side preparation of the project format description for community projects
- requires an extensive configuration
- its application produces output compliant with project metadata requirements!

 \rightarrow Can (but does not have to) be replaced by <u>xarray</u> / <u>NCO</u> in small scale projects

```
cmor_setup();
cmor_dataset_json();
cmor_load_table();
cmor_set_table();
cmor_axis();
cmor_grid();
cmor_set_grid_mapping();
cmor_time_varying_grid_coordinate();
cmor_zfactor();
cmor variable();
cmor_set_deflate();
cmor_set_variable_attribute();
cmor create output path();
cmor_write();
cmor_close();
```

 \rightarrow For large scale projects like CMIP6 (2000+ variables requested for 100+ experiments) there is no way around CMOR!



Project specific data standardization - cdo cmor

Climate Data Operator (CDO) cmor

- CMOR has been integrated into the widely known and commonly appreciated CDOs
- **benefit of CDOs data interface** allowing input in various file formats and structures
- only one call required cdo cmor carries out the complex orchestration of the CMOR functions

Our advice:

Use synergies and profit of cdo CMORs capabilities. Avoid to repeat work by writing your own CMORization tool.

Links

- cdo cmor wiki (incl. User Guide, Hands-On, ...)
- CMIP6 Standardization with cdo cmor extensive <u>Tutorial / Workshop Material</u>
- soon an extensive example to be found here

```
cmor_setup();
cmor_dataset_json();
cmor_load_table();
cmor_set_table();
cmor_axis();
cmor_grid();
cmor_set_grid_mapping();
cmor_time_varying_grid_coordinate();
cmor_zfactor();
cmor variable();
cmor_set_deflate();
cmor_set_variable_attribute();
cmor create output path();
cmor_write();
cmor_close();
```

cdo cmor,Amon ifile.grb



Project specific data standardization - cdo cmor

CMIP6 Amon.json contains parts of the data request in a cdo cmor, CMIP6 Amon.json, \ CMOR-readable format i=.cdocmorinfo, \ mt=mapping table.txt, \ gi=grid info.nc \ infile .cdocmorinfo contains the CMOR configuration activity id="CMIP" institution id="MPI-M"

can be created with https://c6dreq.dkrz.de/cdocmori nfo/index.html grid_info.nc
contains a grid description including
 coordinates and bounds
variables:
 double lat(lat);
 double
lat bnds(lat,bnds);

mapping_table.txt
links model output variables with CMOR variables
¶meter pmt=Amon cmor name=tasmax code=201



Project specific data standardization - Quality Control

<u>PrePARE</u> is distributed with CMOR and checks that the CV and DRS requirements of files are met

PrePARE is the minimal requirement to publish CMIP6 data via the ESGF. At DKRZ we perform additional checks with the Tool <u>QA-DKRZ</u> - a selection of possible checks is listed below:

- folder structure
- compliance with CF conventions
- consistency between different files of the same dataset
- gaps in the timeline (missing files or timesteps)
- outliers

The <u>Jupyter Notebook example</u> contains CMORization examples and a PrePARE check \rightarrow cdo-cmor.ipnb



CMORization - Concluding remarks

- Application of CMOR ensures compliance with project metadata requirements
- Application of NCO / xarray or custom CMOR-like tools ensures weeks of back and forth with the Data Quality Assurance team
- (Setting up the) CMORization takes time and requires efforts and **planning**:
 - We are happy to provide support and to guide you through the CMORization process
 - Please get in touch with us early preferably before starting the simulations:
 - certain output namelist settings might make CMORization much easier
 - for certain output namelists we might have CMORization scripts ready
 - cdo (cmor) might require updates to process your model data
 - \rightarrow If properly planned, CMORization is a manageable task

You can reach us via esgf-publication@dm-rt.dkrz.de



Extra slides



CMIP and **CMOR**

Data standardization means, to rewrite data

- in a common format
- with files structured similarly
- with sufficient and uniformly stored metadata

This is done to enable

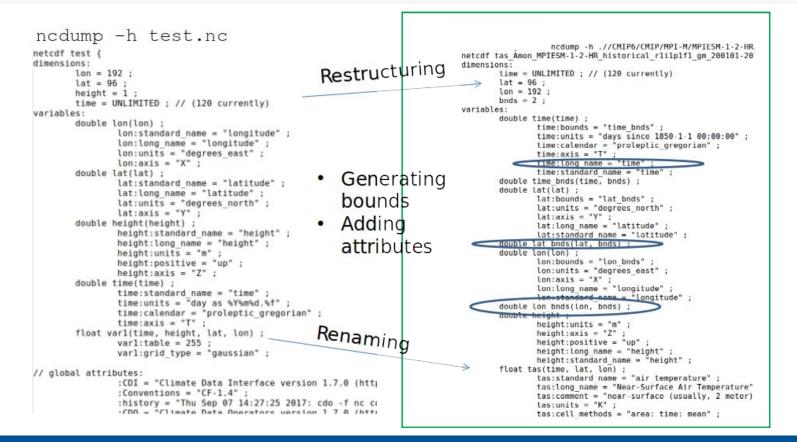
- an easy and fast acquisition or listing of the data (eg. in catalogs or for analysis) with common and widespread tools
- the possibility for intercomparison of data from different sources without requiring complex unit conversions or other post processing steps

Additionally a FAIR publication infrastructure

- quality checks the metadata
- adds identifiers for unique identification and persistent referencing of the datasets
- supports reproducibility of results by keeping track of errata information and retracted / replaced datasets
- ightarrow all only possible due to the standardized (meta)data format and structure



Project specific data standardization



DKRZ User Workshop 2022

Data Standardization



Benefits from the CMIP data infrastructure

Benefits from the CMIP data infrastructure

The CMIP6 data at DKRZ comprises about 4 PB. In order to tackle the challenges of data provision and dissemination for such a repository size, a state-of-the-art data infrastructure has been developed around that pool. In the following, we highlight three aspects of the data workflow.

Data quality

CMIP6 data is only available in a common and reliable Data format

- · No adaptions needed for output of specific models
- · Makes data interoperable and enables general cmip-analysing software products as ESMVal
- CMIP6 data was quality controlled before published with PrePARE
- · We can ensure e.g. correct coordinates and attribute configurations in the data

CMIP6 data is transparent about occuring errors

· Search the errata data base for origins of suspicious analysis results

Data publication

- · Find and access data via the fail-safe ESGF portal due to the redundant network of ESGF nodes
- . Exentended documentation for simulation conducts provided in the ES-Doc data base
- · Persistent Identifier (PIDs) ensure long-term webaccess to dataset information
- Citation information and DOIs for all published datasets easily retrievable

Data curation

The CMIP6 data pool is maintained by

- · automatic ingest and egest which keeps the data updated
- · Back ups of the data pool in the tape archive
- · Long term archival for a range of datasets used in the IPCC report

⇒ High quality Analysis services only because of a high quality data supply

Keep Acknowledging and requesting high data quality!



Other jupyther notebooks

Notebooks der summer school:

netcdf basics https://github.com/IS-ENES-Data/summer-school-2022/blob/main/notebooks/files_and_to ols/NetCDF%20and%20CF%20-%20The%20Basics.ipynb

xarray basics: https://github.com/IS-ENES-Data/summer-school-2022/blob/main/notebooks/files_and_to ols/XArray%20and%20CF.ipynb

nco ncdump cdo basics: https://github.com/IS-ENES-Data/summer-school-2022/blob/main/notebooks/files_and_to ols/basic_netcdf_utils.ipynb

xarray (with cf-xarray part): https://github.com/IS-ENES-Data/summer-school-2022/blob/main/notebooks/files_and_to ols/xarray-in-45-min.ipynb

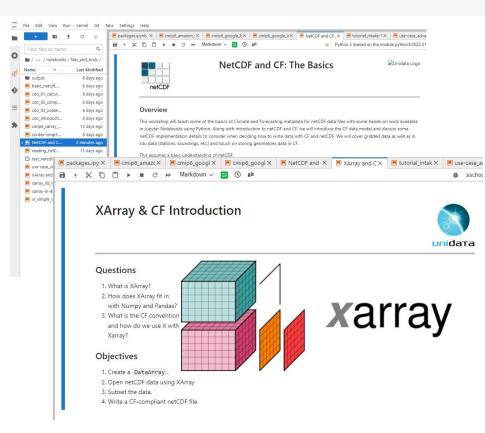


CMIP and CMOR

Hands on examples for NetCDF-CF:

- NetCDF and CF The Basics.ipynb
 - shortend version of notebook from <u>Unidata training material</u> repo
 - uses netCDF4-python library

- XArray and CF.ipynb
 - from <u>Unidata workshop training material</u> repo
- if you are not yet familiar with xarray please get back to this after the next session where xarray basics will be introduced ..





Elements of CF-netCDF

Element	Description
Data variable	Scientific data discretised within a domain
Dimension	Independent axis of the domain
Coordinate variable	Unique coordinates for a single axis
Auxiliary coordinate variable	Additional/alternative coordinates for any axes
Boundary variable	Cell vertices
Ancillary data variable	Metadata that depends on the domain
Formula terms attribute	Vertical coordinate system
Feature type attribute	Characteristics of discrete sampling geometry
Cell methods attribute	Description of variation within cells

