

Barcelona Supercomputing Center Centro Nacional de Supercomputación



Data quality assurance: general overview and the EC-Earth case

PA Bretonnière, EC-Earth meeting, 21/05/2019

Outline

- 1. Quality Assurance overview
 - a. Why checking the data?
 - b. Sources of errors
 - c. What is a good dataset?
- 2. QA project and software inventory
 - a. C3S512
 - b. Existing data checkers
- 3. What about EC-Earth?
 - a. Current status
 - b. Roadmap for developments



- 1. Increase trustability
- 2. Avoid making wrong scientific decisions
- 3. Long simulation times imply non rerunnable
- 4. Avoid having to exchange long emails to clarify data issues:



- 1. Increase trustability
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From					21.50	elete	More	~
To	le			1 mo	21.59		22	2:01
Hi,								

I'm loading the data downloaded from xxxxx and even if metadata say it's an average, it looks like instantaneous values, can you confirm that everything is OK please?



Thank you, Best regards,

Quality Assurance overview a. Why checking the data? b. Potential sources of errors c. What is a good dataset?

- 2. QA project and software inventorya. C3S512b. Existing data checkers
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QA overview: sources of "errors"

1. Hardware or system tools failures -> data corruption

- (s)cp errors, file system failure during writing,...:
 - ncdump: myfile.nc: NetCDF: Unknown file format
 - GRIB_API ERROR : unable to create index for input file ICMGGa1i2+196001 (Wrong message length)
- 2. Workflow errors -> the data is not what we expect it to be
 - cmor done before leg+1 resulting in missing timestep
 - rerun on existing files -> extra timesteps in grib
- 3. Software bugs -> we don't produce what we think we do
 - date in the files is not what we expect



QA overview: sources of "errors"

- 4. User configuration mistakes -> we don't produce what we are supposed to
 - wrong forcing files are read
 - wrong variables/frequencies in varlists
- 5. "Scientific configuration" of the model/experiment
 - pptd is not well written
 - mask is not read correctly



1. Quality Assurance overview

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What is a good dataset?





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C3S_512: QA for the Climate Data Store

- Objective:
 - Providing a user-led overarching EQC service for the whole CDS
 - Providing an independent quality assessment for a number of data types (seasonal forecasts, climate projections and in-situ observations)
- Participants:
 - BSC, DWD, FMI, KNMI, Météo-France, Predictia, CNR, WENR





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C3S_512: QA for the Climate Data Store

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	Please	note that some ERA5 download	is might occassionally fail due	e to internal system issues. P	ease contact user supp	ort for further i	nformation.	
verview Download data	Documentation					_	Contact copernicus-support@ecmwf.in/	t
Variable ⑦ At least one selection must be m Temperature V-component of wind Relative humidity	iade		U-component of wir Specific humidity Geopotential height	d			License CMIP5 - Data Access - Terms of Publication Date	Use
Model ⑦ At least one selection must be m inmcm4 (INM, Russia) bcc-csm1-1 (BCC, China) BNU-ESM (BNU, China) CNRM-CM5 (CNRM-CERFAC GFDL-ESM2G (NOAA, USA) GISS-E2-H (NASA, USA) GISS-E2-R (NASA, USA) GISS-E2-R (NASA, USA) GISS-E2-R (NASA, USA) HadGEM2-CC (UK Met Offic IPSL-CMSB-LR (IPSL, France; IPSL-CMSB-LR (IPSL, France;	ade CS, France) :e, UK))		ACCESS1-0 (BoM-CS bcc-csm1-1-m (BCC, CMCC-CMS (CMCC.) GFDL-CM3 (NOAA, U GFDL-ESM2M (NOA4 GISS-E2-H-CC (NASA GISS-E2-R-CC (NASA HadGEM2-ES (UK M PISL-CMSA-MR (IPSL MPI-ESM-LR (MPI, G	RO, Australia) China) taly) SA) , USA) , USA) , USA) et Office, UK) , France) rrmany)			Related data CMIP5 daily data on pressure le CMIP5 monthly data on single le CMIP5 daily data on single level	evels evels Is
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Ensemble member 🔊								



C3S_512: QA for the Climate Data Store

• Main QA tasks: for each data type

- develop a data checker checking the minimum requirements:
 - file integrity
 - grib keys
 - valid ranges
 - ensemble spread
 - time completeness
- develop softwares able to do automatic scientific assessment of the data computing different metrics:
 - skill scores
 - RMSE
 - FairRPSS



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- CF checker:
 - Developed by: CEDA
 - Run in: command line and "drag and drop"
 - **Type of file checked:** netcdf
 - **Checks:** units, standard/long names, dimensions
 - Reference: CF conventions (html)



Supercomput

<u>http://pumatest.nerc.ac.uk/cgi-bin/cf-checker.pl</u>
<u>https://github.com/cedadev/cf-checker</u>

- PrePARE:
 - Developed by: PCMDI
 - Run in: command line
 - □ **Type of file checked:** CMIP6 netCDF
 - Checks: file names and metadata
 - Reference: MIP tables

Link(s): <u>https://cmor.llnl.gov/mydoc_cmip6_validator/</u>



- ESMValTool
 - Developed by: DLR, AWI, BSC, NLeSC, Ludwig Maximilian University of Munich, University of Reading
 - Run in: through python jobs
 - □ **Type of file checked:** netcdf "CMOR-like"
 - Checks: metadata compliance
 - Reference: MIP tables





https://github.com/ESMValGroup/ESMValTool

- UKCP18-CC
 - Developed by: CEDA
 - Run in: command line
 - **Type of file checked:** netcdf
 - Checks: file and directory structure, metadata compliance,...
 - **Reference:** rules from user defined json files



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https://github.com/ukcp-data/cc-plugin-ukcp18

- nctime:
 - Developed by: IPSL
 - Run in: command line
 - **Type of file checked:** netcdf CMIP6 CMOR
 - **Checks:** time completion of set of files, time "validity"
 - Reference: N/A

Link(s): <u>https://github.com/Prodiguer/nctime</u>



- C3S512 grib checker (under development):
 - Developed by: BSC
 - Run in: command line
 - Type of file checked: CDS grib files (model and reanalysis)
 - **Checks:** grib keys, ensemble spread, valid ranges,
 - Reference: grib tables, MIP tables
 - Link(s):



https://earth.bsc.es/gitlab/ces/c3s512-wp1-datach

- PRIMAVERA checker
 - Developed by: CEDA
 - Run in: command line
 - **Type of file checked:** netCDF CMOR PRIMAVERA
 - **Checks:** metadata, time coherency, file integrity
 - Reference: MIP tables,...



- and more:
 - CMOR
 - check-nemo-files (Klaus Zimmermann)
 - QA-DKRZ



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• What do we (currently, operationally, automatically) check?



What do we (currently, operationally, automatically) check?
 o at the consortium level: (almost) NOTHING!





- What do we (currently, operationally and automatically) check?
 - at the institute level:
 - CMORization/ece2cmor (all, online or offline)
 - "some checks" for NaN on Nemo files (SMHI)
 - "some checks" on CMOR files (CNR)
 - "some checks" on grib files (BSC)
 - "more extensive checks" on pre-ESGF publication (BSC)
 - more?



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• Check "original/raw" and CMOR files





Check "original/raw" and CMOR files grib_dump cdo info 0





Check "original/raw" and CMOR files

- ece2cmor/CMOR \bigcirc
- PREPARE \bigcirc
- UKCP18-CC \bigcirc



Informatics



- Check "original/raw" and CMOR files
 - o cdo/nco
 - check_nemo_files



Informatics



Check "original/raw" and CMOR files

 ???
 nctime



Informatics



Check "original/raw" and CMOR files

 C3S_512 grib_checker
 ece2cmor/CMOR



Informatics



Check "original/raw" and CMOR files





Conclusions

- It is impossible to QA everything automatically but there is room for improvement
- Possible checks to be implemented:
 - file corruption for raw IFS and Nemo
 - timesteps/date coherence for raw IFS and Nemo and CMOR files
 - masks and NaN for Nemo raw files
 - variable list completeness for CMOR files
 - metadata coherency for CMOR files (PrePARE)
 - **time completeness** for CMOR files (nctime)





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Thank you

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