

CMIP6 Data Management at DKRZ

iCAS2015

Annecy, France on 13–17 September 2015

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With contributions from ESGF Executive
Committee and WGCM Infrastructure Panel

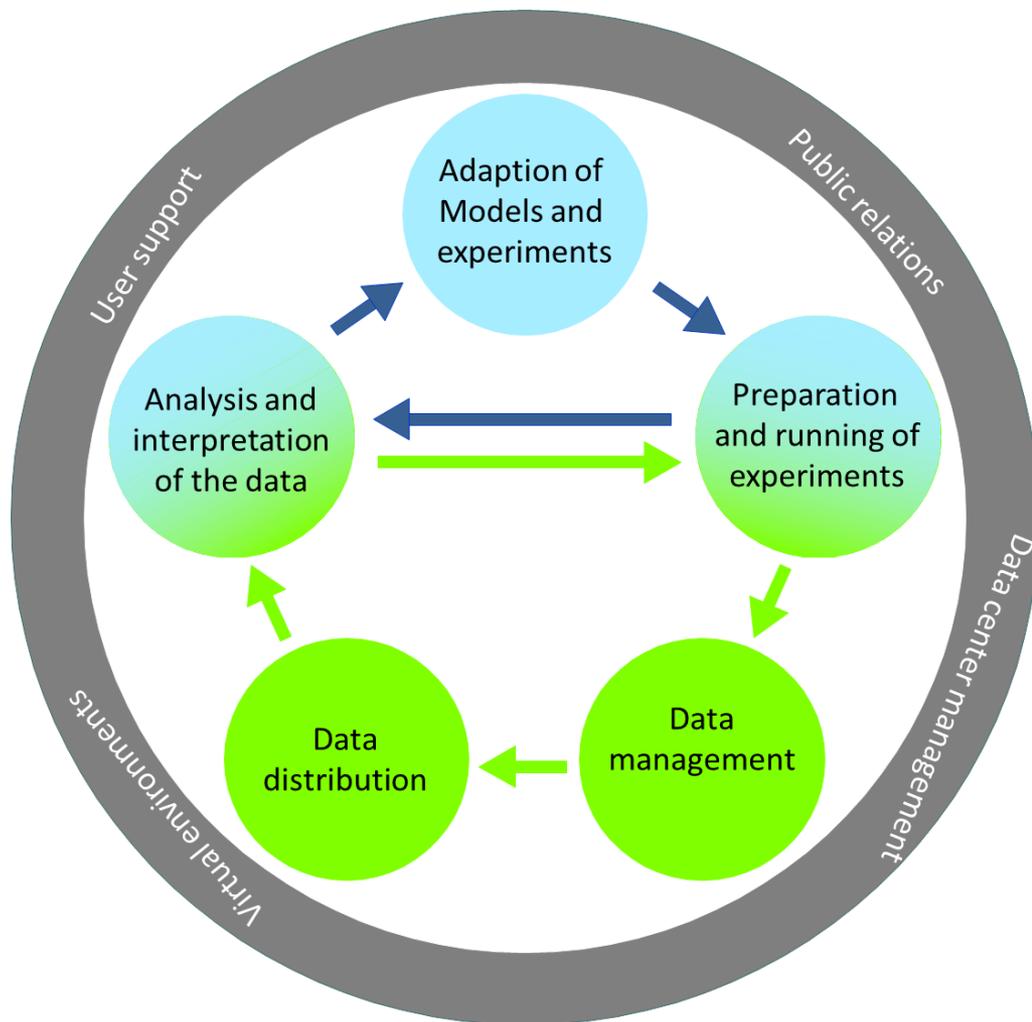
CMIP6 Data Infrastructure at DKRZ

<http://www.dkrz.de/Klimarechner-en/hpc/hlre-3-mistral>

- HLRE-3: Next HPC generation at DKRZ in operation since July 2015
 - More details by Joachim Biercamp on Wednesday afternoon
- CMIP6 resources will be integrated into the HPC system
 - Compute: several compute nodes for ESGF, postprocessing and visualisation
 - Disk Space: 1.5 – 2 PB in addition to HLRE-3
 - Tape space: 30 – 50 PB in addition for long-term archiving
 - Network connection: 2 times 10 Gbit/s



DKRZ Service Structure



Basic workflows:

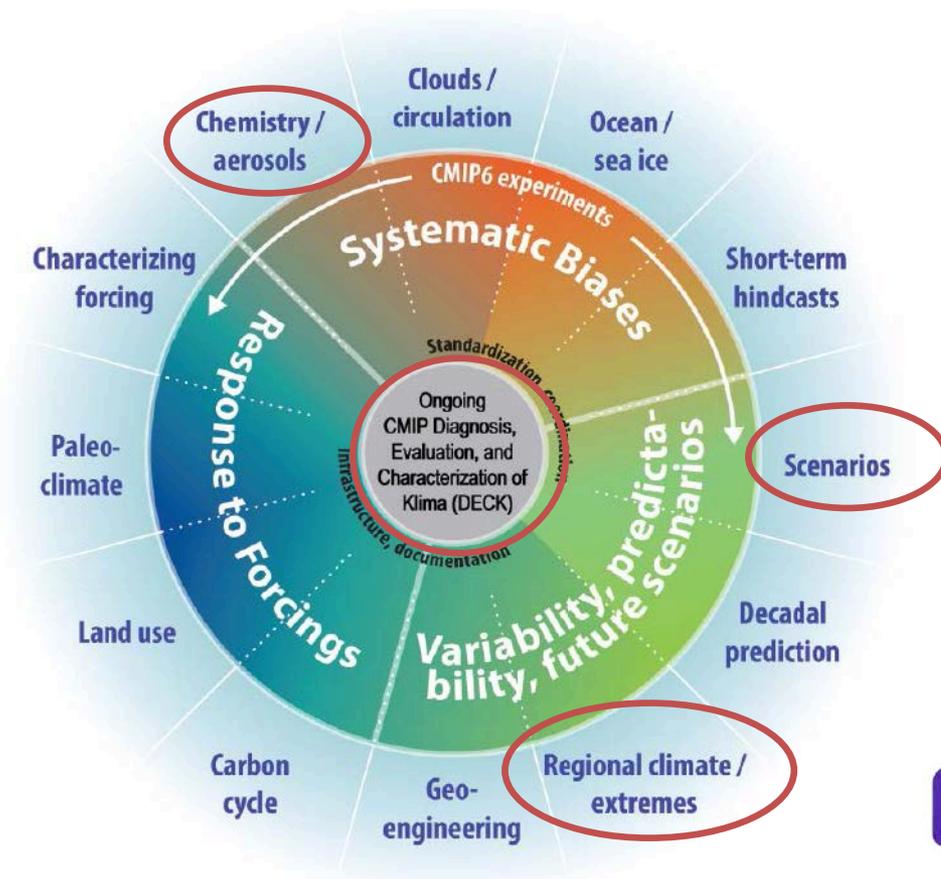
Climate Model Development

Climate Model Data Production

CMIP6

CMIP6 Experiment Structure

CMIP6



Focus of DKRZ:

Probably CMIP6 funding from BMBF to support

- DECK (Diagnosis, Evaluation and Characterization of Klima)
- Scenarios
- Regional Climate / extremes
- Chemistry / aerosols

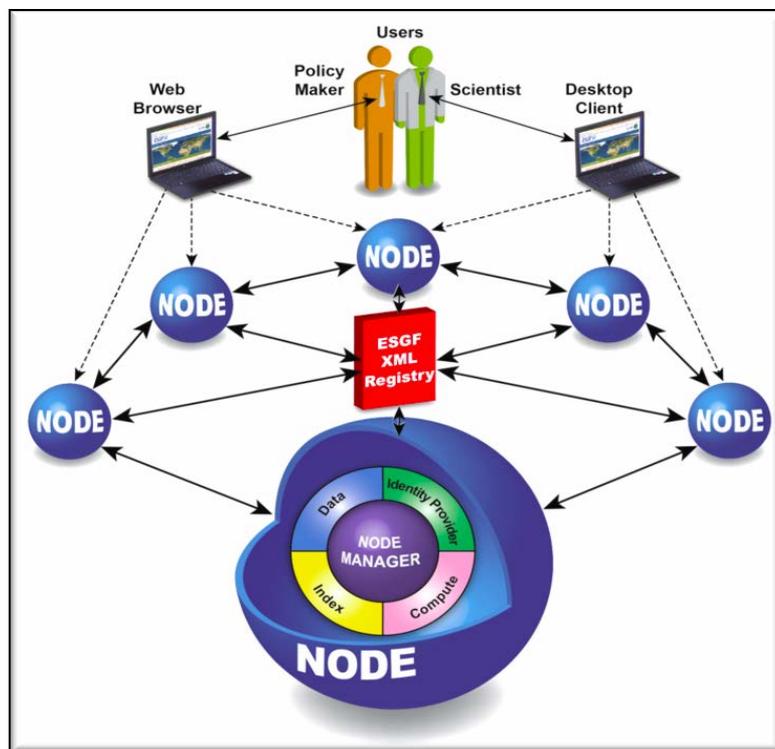


CMIP6 Data Volume Estimate

- **Status CMIP5 data archive (June 2013)** as presented in iCAS2013:
 - 1.8 PB for 59000 data sets stored in 4.3 Mio Files in 23 ESGF data nodes
 - CMIP5 data is **about 50 times** CMIP3
- **Extrapolation to CMIP6:**
 - CMIP6 has a more complex experiment structure than CMIP5.
 - Expectations: more models, finer spatial resolution and larger ensembles
 - **Factor of 20:** 36 PB in 86 Mio Files
 - **Factor of 50:** 90 PB in 215 Mio Files
 - More accurate numbers after the modelling groups CMIP6 survey starting in October 2015

CMIP6 Data Infrastructure

ESGF is a software infrastructure for management, dissemination, and analysis of simulation and observational data. The software utilizes hardware, networks, software for data management, access and processing.



ESGF federation nodes interact as equals. Users log onto any node using single sign-on OpenID to obtain and access data throughout the entire federation.

Lessons learned: CMIP5 Summary from iCAS2013

- ESGF started to **analyse the CMIP5 experiences** in order to improve the ESGF data infrastructure:
 - Managing large data archives is not only a technical problem.
 - The establishment of a stable distributed ESGF infrastructure requires stable commitments and funding
- ESGF has **requests from alternative modelling efforts** and related observations to be included in ESGF in order to have all these data more easily inter-comparable.
- Federated data infrastructures like ESGF or Data Clouds seem the way to go for the **next generation of climate data archives**
 - CMIP5 to CMIP6: $1.8 \text{ PB} * 50 = 90 \text{ PB}$ for one these MIPS
- **Requested improvements**
 - Usability of ESGF data access interface
 - Automated data replication between ESGF data nodes
 - More powerful, more stable and scalable wide area data networks (service level agreements)
- More details from CMIP6 web pages:
http://www.wcrp-climate.org/images/modelling/WGCM/CMIP/SynthesisCMIP5Survey_131001.pdf



Not the most important aspect

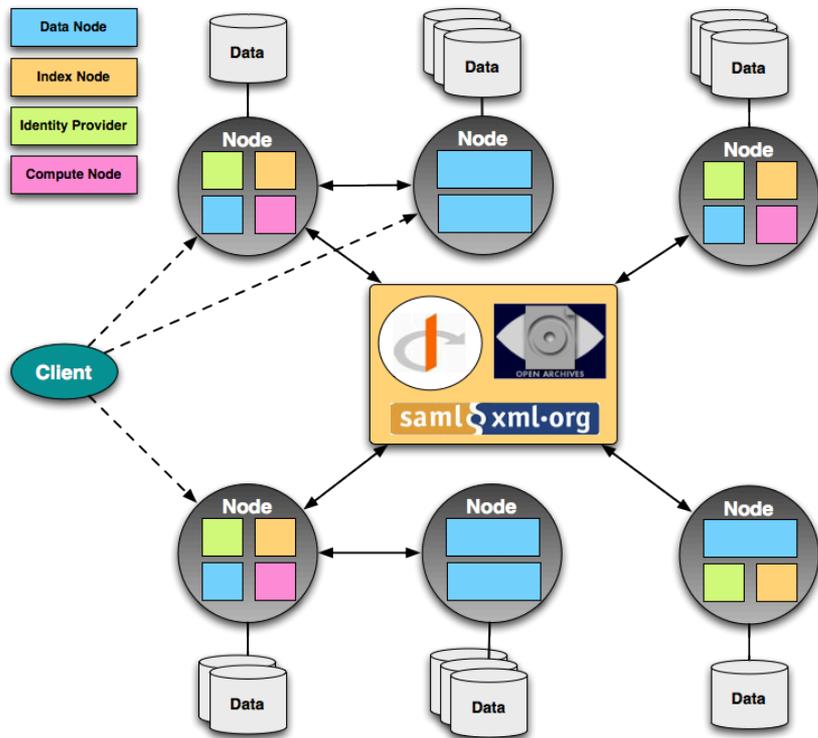
CMIP6 Implementation

Discussions in 2014/15 in and between WCRP/WGCM, CMIP Panel and ESGF Development led to a clear separation between

- ESGF as data infrastructure
 - ESGF governance process
 - CMIP6 is one (large) data project among others
 - Clear separation between ESGF governance process and scientific data project management like CMIP6

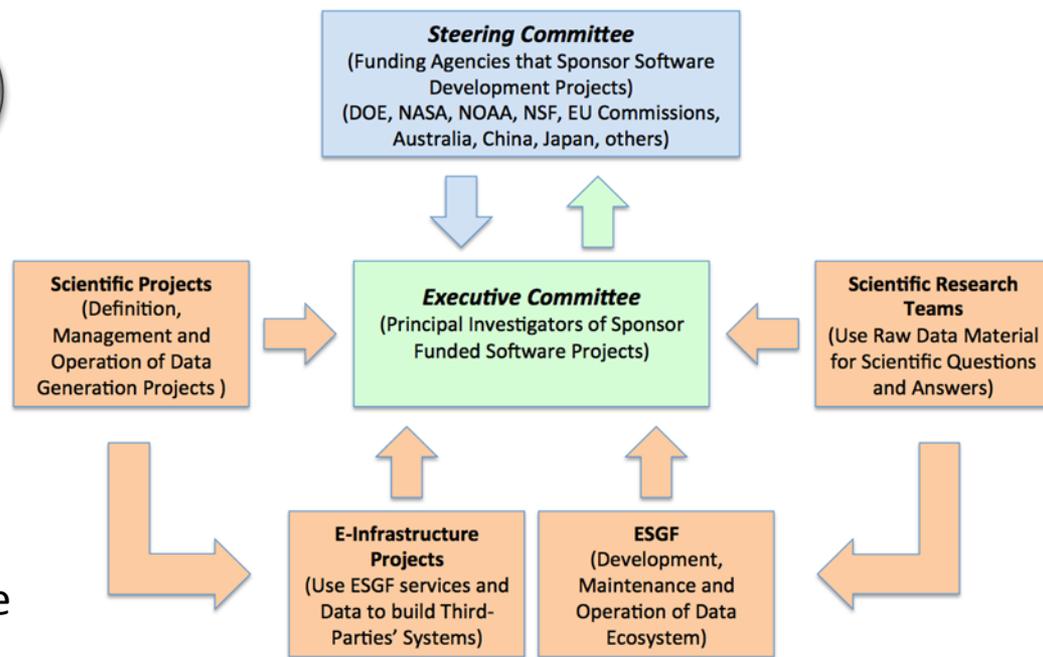
- CMIP6 scientific data management
 - WIP (WGCM Infrastructure Panel) for data management
 - Series of white papers to specify management principles

ESGF as CMIP6 Data Infrastructure



ESGF's federation architecture is based on modular components and standard protocols.

The ESGF Governance Communication Architecture



CMIP6 Data Management

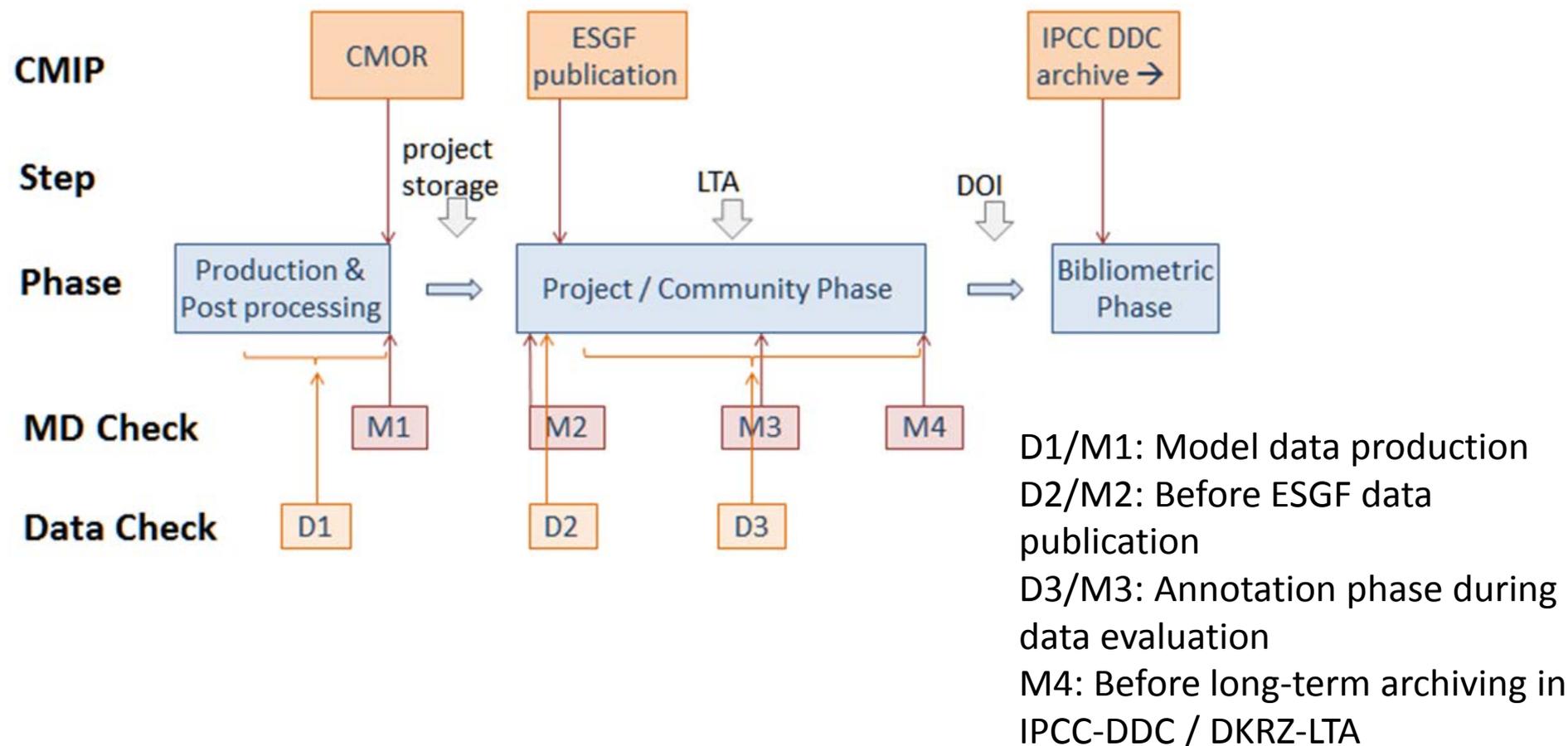
- WIP action items from [WCRP/WGCM-18 meeting, Oct. 2014](#)
 - Standards to describe climate models and their forcings (ESDOC / CIM)
 - Stability of DRS (Data Reference Syntax) and CMOR (Climate Model Output Rewriter)
 - Early data citation reference to give credit to modelling groups
 - Management of CMIP6 data requests
 - Guidance to MIPs about coordination of standards
 - Some management of data volume

- This resulted in a list of [WIP White Papers](#) on
 - Replication and Versioning (**DKRZ focus**) (d)
 - Use of Persistent Identifiers (**DKRZ focus**) (b)
 - Data Reference Vocabularies
 - Data Request Structure and Process
 - Data Quality Assurance (**DKRZ focus**) (a)
 - Data Citation and Long-term Archiving (**DKRZ focus**) (c) (e)
 - File Names and Global Attributes
 - Licensing and Access Control

- Network improvement / ICNWWG (f)

Data Quality Assurance (DM + ESGF)

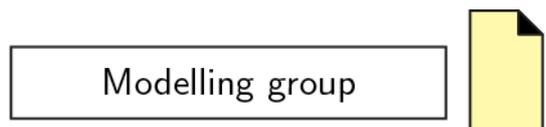
- Impact on CMIP6 data management (DM) and ESGF governance (ESGF)
- CMIP6 workflow refers to the different stages in the data life cycle:



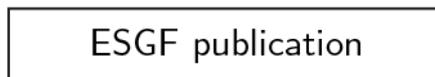
Use of Persistent Identifiers (DM + ESGF)

- Impact on CMIP6 data management (DM) and ESGF governance (ESGF)
- CNRI Handle System PIDs assigned to NetCDF files and data collections (atomic data sets, simulations and models)
- PID publication workflow:

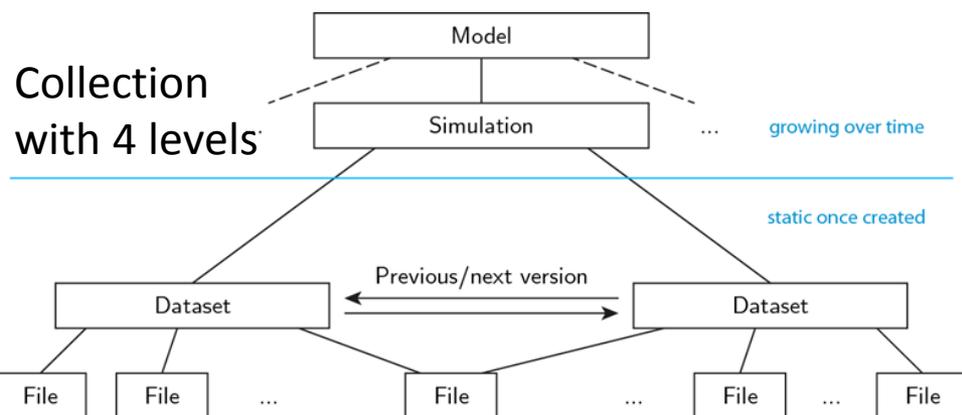
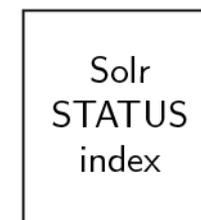
(CMOR)



- ✓ PID tracking_ID syntax correct
- ✓ Citation information complete

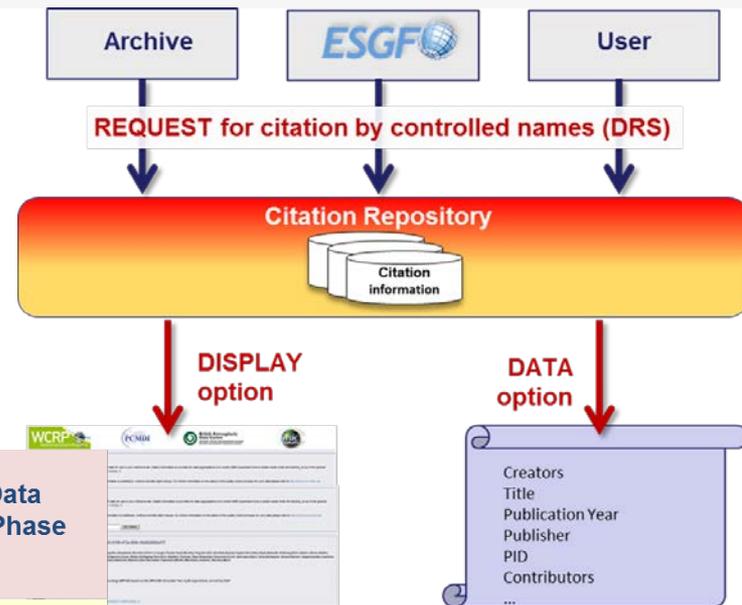


- PIDs registration →
- Citation information confirmation →
- File publication →



(Early) Data Citation (DM + ESGF)

- Impact on CMIP6 data management (DM) and ESGF governance (ESGF)
- Request from modelling groups for a data citation reference together with ESGF data publication
- CMIP6 data publication workflow:



Paper Publication	Data Publication	Data Workflow	
	Data partly available	ESGF publication of initial (incomplete) data	Initial Data Sharing Phase
Paper Preparation	Data Analyses		
Draft Paper Publication	Early Data Publication	ESGF publication of Revised Datasets as new versions and withdrawal of old versions	Data Review Phase
Paper Peer-Review	Data Community Review		
Final Paper Publication (Early Data Citations)			
Final Paper Publication (DataCite DOI Data Citations)	LTA Data Publication	Data is finalized, long-term archived, and DataCite DOI Published	Stable Data Phase

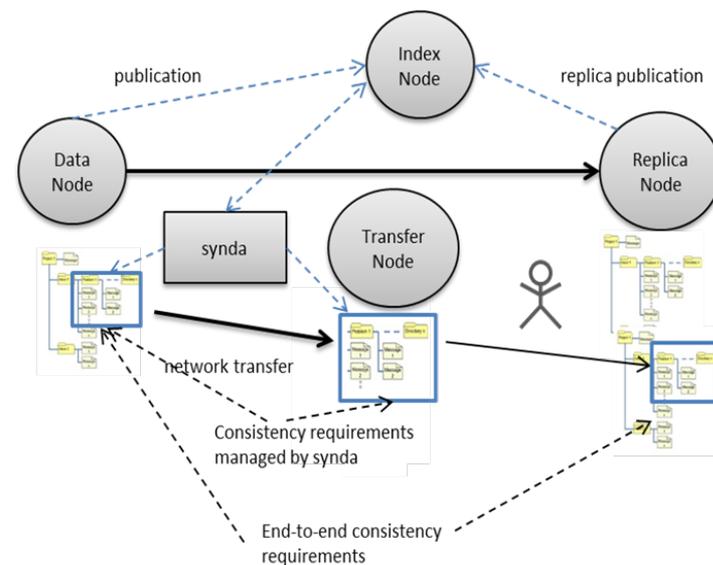
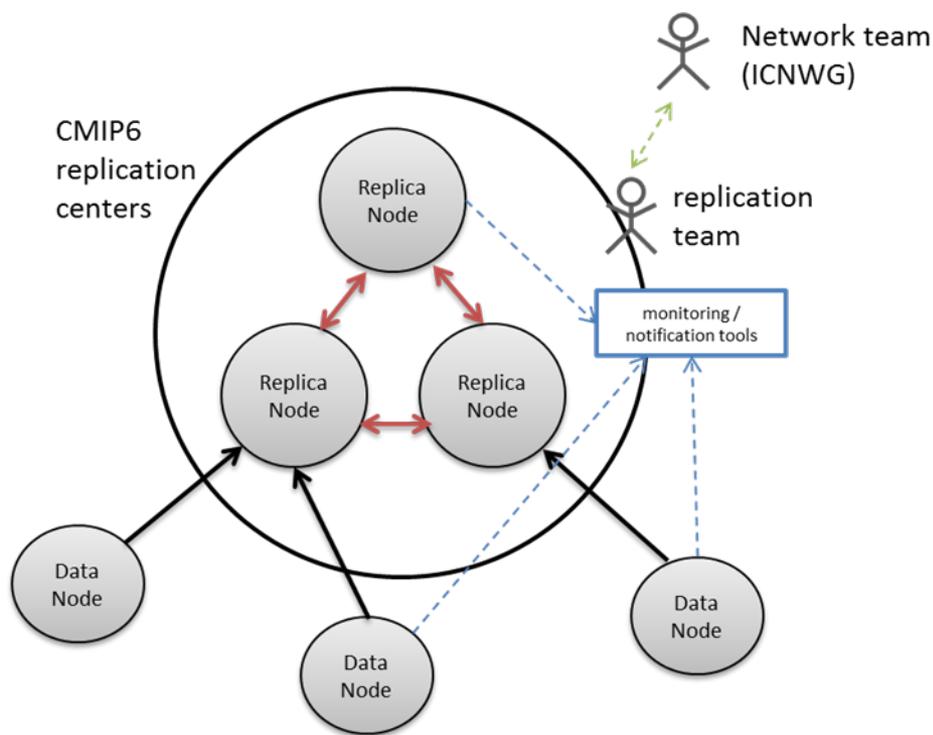
Time ↓

CMIP6 citation granularities are collection levels:

- Simulation**
- Model**

Replication and Versioning (DM + ESGF)

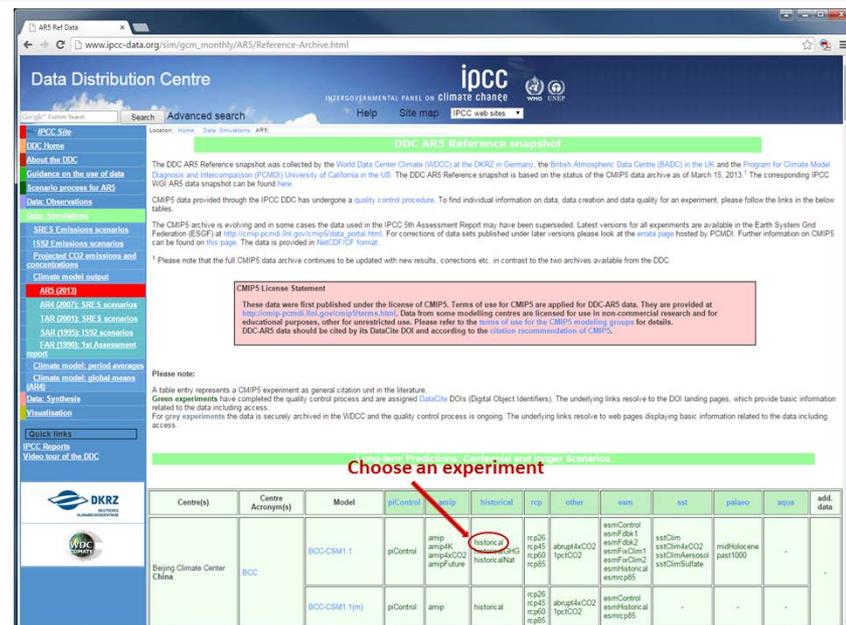
- Impact on CMIP6 data management (DM) and ESGF governance (ESGF)
- Stable processes which are supervised by a board (the CDNOT Team) are needed for CMIP6 data consistency in ESGF
- CMIP6 data replication architecture:



CMIP6 replication procedure

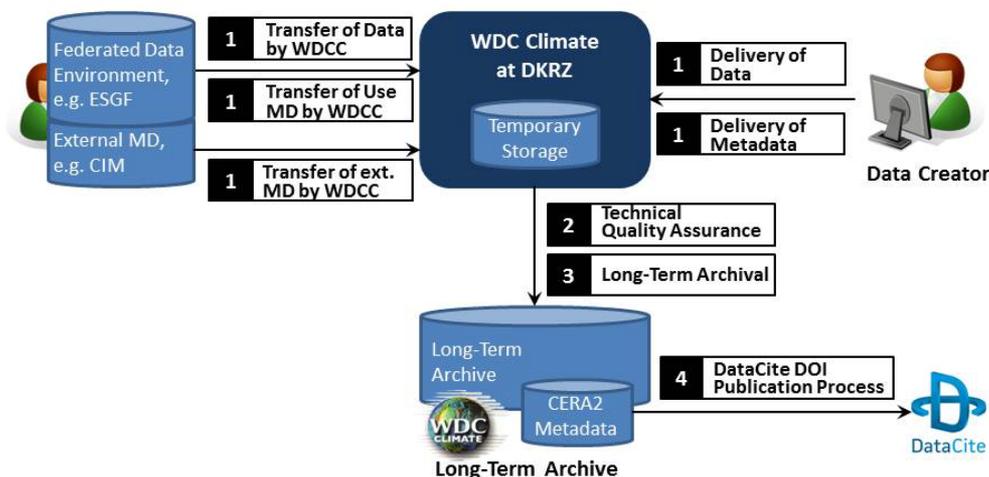
Long-term Archiving as for CMIP5

- Nothing new for CMIP6 compared to CMIP5 except the increased data volume, number of data entities and more complex external metadata
- IPCC AR6 reference data will be transferred into the IPCC DDC for long-term archiving together with their DataCite data publication



Federated Projects
e.g. CMIP6

DKRZ or Central Projects



IPCC DDC

- DKRZ: Long-term archiving of GCM data in DKRZ-LTA (30 – 50 PB)
- BADC: Operation of Web-server including documentation, guidance material and visualisation

ICNWG and Network Improvement (ESGF)

- Impact on ESGF governance (ESGF) by stabilizing networks and optimise throughput
- ICNWG (International Climate Network Working Group) is one of 18 ESGF development working groups
- Basic result: Network performance is often limited by end systems than by wide area network
- ICNWG site map (minimum connection bandwidth 10 Gbit/s [~ 1 GB/s]):

Average data rates for a single 50 GB file and for 50 GB set of 1875 small files of 10 – 50 MB (May 2015):

NCI: 300 / 300 (excessive parallelism)

CEDA: 200 / 6 (170 with CERN)

DKRZ: 350 / 40

Measures are in MB/s



Test shows that for the single file case **1/3 of the nominal bandwidth** could be realised.

Next steps: data transfer optimisation for CMIP5 climate model data with 240 GB data sets consisting huge files (more than 100 GB), large files (10 – 100 GB), medium files (1 – 10 GB) and small files (less than 1 GB)

Summary

- CMIP6 data management improvements based on CMIP5 experiences
 - *Infrastructure*: data publication, versioning/replication, access, identification and citation
 - *Organisation*: ESGF governance, WGCM infrastructure panel (WIP), end user community gets more diverse and is growing
 - ESGF Software Security Working Team is solely dedicated to the integrity of the software stack.
- DKRZ focus on managing curated CMIP6 data collections
 - Quality assurance, data identification and citation
 - Handle PIDs to find and to reference data objects over their life cycle independently from their actual storage location
 - Early Citation reference for structured climate data citation at the very beginning of the data life cycle
 - Replication, versioning and network
 - Tests in the ICNWG have shown that the **wide area networks are often not the impediment to performance**, but rather the problem is the configuration of the end systems (e.g. storage, data transfer nodes), and the configuration of the local networks (firewalls, underpowered switches, etc).
 - Preparing for “near data processing” challenge
 - “download and process at home approach” for data analysis gets more and more problematic

Aspects which are not covered here

List of aspects which are not covered in this presentation but which are in process in ESGF working groups and in the WIP:

- CMOR (Climate Model Output Rewriter) (DM)
- Vocabularies (DM)
- DRS (Data Reference Syntax) (DM)
- CIM (Climate Information Model) (ESGF + DM)
- Errata and annotations (ESGF + DM)
- Licensing (DM)
- GUI (ESGF)
- AAI (ESGF)
- Near data processing (ESGF + DM)



ESGF: <http://esgf.llnl.gov/>

WIP / WGCM: <https://earthsystemcog.org/projects/wip/>