Evolution and Future Architecture for the Earth System Grid Federation

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Introduction

The Earth System Grid Federation (ESGF) is a globally distributed e-infrastructure for the hosting and dissemination of climate-related data.

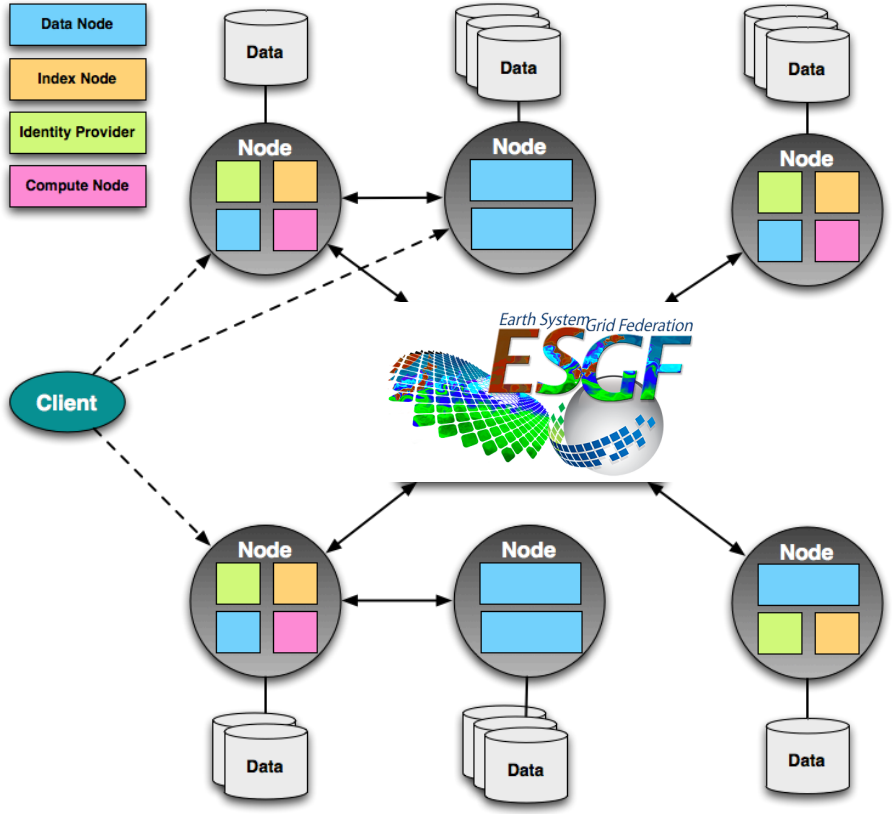
ESGF was originally developed to support CMIP5 (5th Coupled Model Intercomparison Project) …

Provide a means for climate research community to access and analyse the data output

For 5th Assessment report made by the IPCC (Intergovernmental Panel on Climate Change).

Ten years of Operations: History and Evolution

- ESGF has grown to support over
  - 25000 registered users
  - 33 registered nodes at climate research centres spread across 21 countries, sites including DoE, EU IS-ENES collaboration, NASA, NOAA, NCI Australia …
- Besides the CMIPs, supports a range of other projects such as the Energy Exascale Earth System Model, Obs4MIPS, CORDEX and the European Space Agency's Climate Change Initiative Open Data Portal.
- Over the course of its evolution, ESGF has pioneered technologies and operational practice for distributed systems
  - Federation inherently supports redundancy and large-scale data replication capabilities
  - Search, metadata modelling and capture, identity management
- Important experience gathered over the years about community collaboration for a distributed infrastructure - operational procedures and governance



Federation stats: ESGF Dashboard

Published data over the federation

Current values

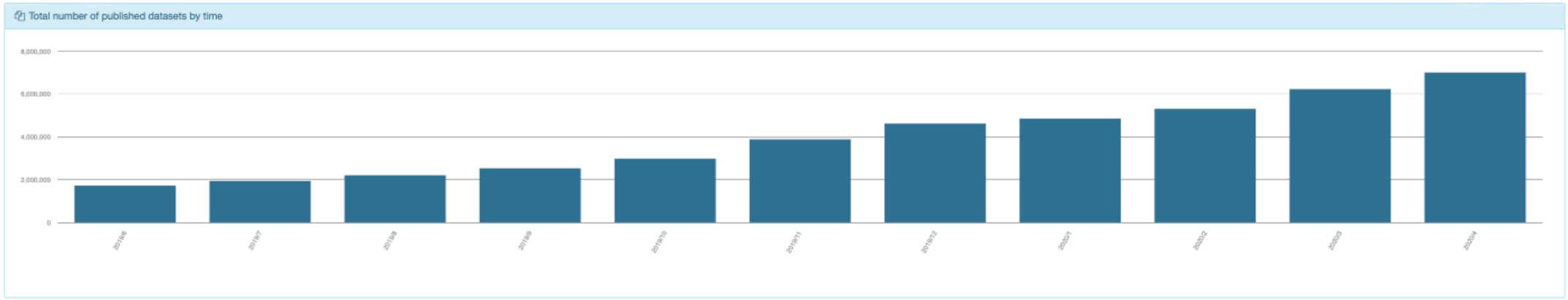
2,283,135 total datasets
7,948 TB

2,013,388 distinct datasets
5,176.93 TB

269,747 replica datasets
2,771.08 TB

Published data over time (updated every first day of the month)

Total datasets number | Total data size [TB] | CMIP6 Datasets number | CMIP6 Data size [TB] | CORDEX Datasets number | CORDEX Data size [TB]



Top projects (updated daily)

CMIP5	206,604 total datasets 5,484.38 TB	CMIP5	25,750 distinct datasets 796.75 TB	CMIP5	70,020 replica datasets 1,596.25 TB
CMIP6	1,540,435 total datasets 5,071.62 TB	CMIP6	1,340,732 distinct datasets 3,897.44 TB	CMIP6	199,703 replica datasets 1,174.18 TB
INPUT4MIPS	11,311 total datasets 19.82 TB	INPUT4MIPS	5,660 distinct datasets 9.97 TB	INPUT4MIPS	5,651 replica datasets 9.86 TB
OBS4MIPS	93 total datasets 0.28 TB	OBS4MIPS	93 distinct datasets 0.28 TB	OBS4MIPS	0 replica datasets 0 TB
CORDEX	83,687 total datasets 280.99 TB	CORDEX	83,687 distinct datasets 280.99 TB	CORDEX	0 replica datasets 0 TB

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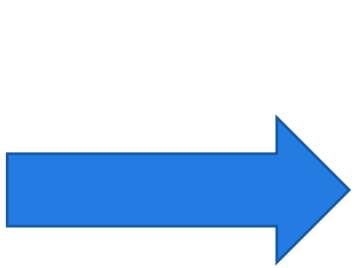
Big Data, cloud and the evolution of systems for data distribution and analysis

Big Data driving changes in architecture



Single data centre

- Discover and download user model
- non-federated data repositories

Federated data repositories

- Multiple organisations
- geographically distributed download capability
- **Earth System Grid Federation** initially for **CMIP5 Global Climate Projections** from 2008

Public Cloud

- Content Delivery Network

Data analysis facility

- Co-located compute and data
- Bring the compute to the data paradigm
- NCI Australia (2010)
- JASMIN (2012)

Data Analysis Platforms

- Co-located compute and data
- High Performance Data (HPD), Analysis Ready Data (ARD)
- Community Resources
- ESA Thematic Exploitation Platforms

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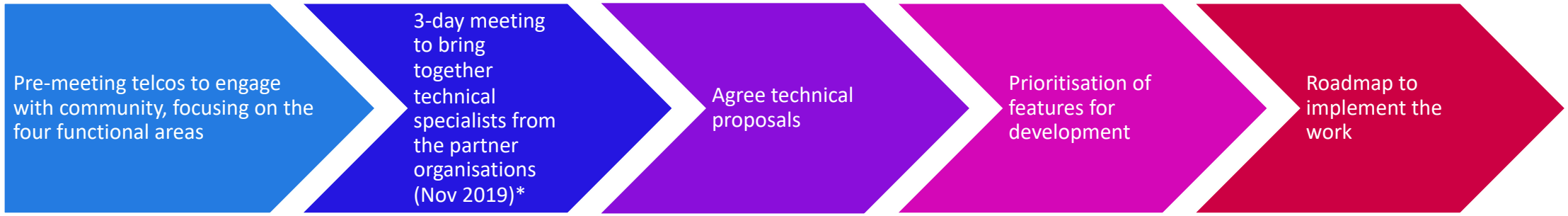
Future Architecture

- An initiative to re-design ESGF
- Drawing from our experience and lessons learnt
  - running ESGF operationally and
  - other large-scale compute/data systems at our facilities
- Also considering other similar systems and initiatives e.g.
  - Interoperable community standards – ISO Catalogues, OpenSearch, FAIR, schema.org, RDA …
  - ESA's Earth Observation Exploitation Platform Common Architecture (https://eoepca.github.io)
  - OGC Testbeds
  - Pangeo (https://pangeo.io/), a community and software stack for the geosciences

High-Level Functional Areas to Consider

1) User Experience
2) Data Repository and Management
3) Compute on Data
4) Platforms and systems administration

Approach



* Report write-up of the above

Findings

- User Experience
  - Need more integrated search across all data holdings: integrate metadata about models (ES-Doc system) as well as netCDF metadata
- Data Repository and Management
  - Develop new publishing system and adopt new search API standard (later slide)
  - New approach needed over traditional data access mechanisms such as OPeNDAP. Desire for new and efficient means for sub-setting and aggregation
- Platforms and systems administration
  - Strong consensus to build on work to standardize deployment based on Docker and Kubernetes
  - Make architecture more modular with clearly defined interfaces
  - This will better facilitate contributions from the development community
- Compute on Data
  - No consensus to standardize on a single federation-wide reference implementation
  - However, plenty of individual projects leveraging ESGF developing processing services based on OGC Web Processing Service standard
  - These include work tying in with recent OGC Testbeds
  - Individual sites are also deploying services based on Python stacks with Jupyter
- More findings …

Federation or Cloud for Resilience?

Federation allows scaling, redundancy, sharing of capability

Search and identity management are the linchpins of federation

But federation can also bring complexity:

- Search and identity management services are duplicated across sites
- There can be a high operational burden
- Duplication of services can be confusing for users

Cloud computing with its impact on deployment practice and hosting architecture can help

Public cloud with 4 9s resilience capability brings back centralisation as a viable design choice vs. the previously established approach in ESGF of federation for resilience

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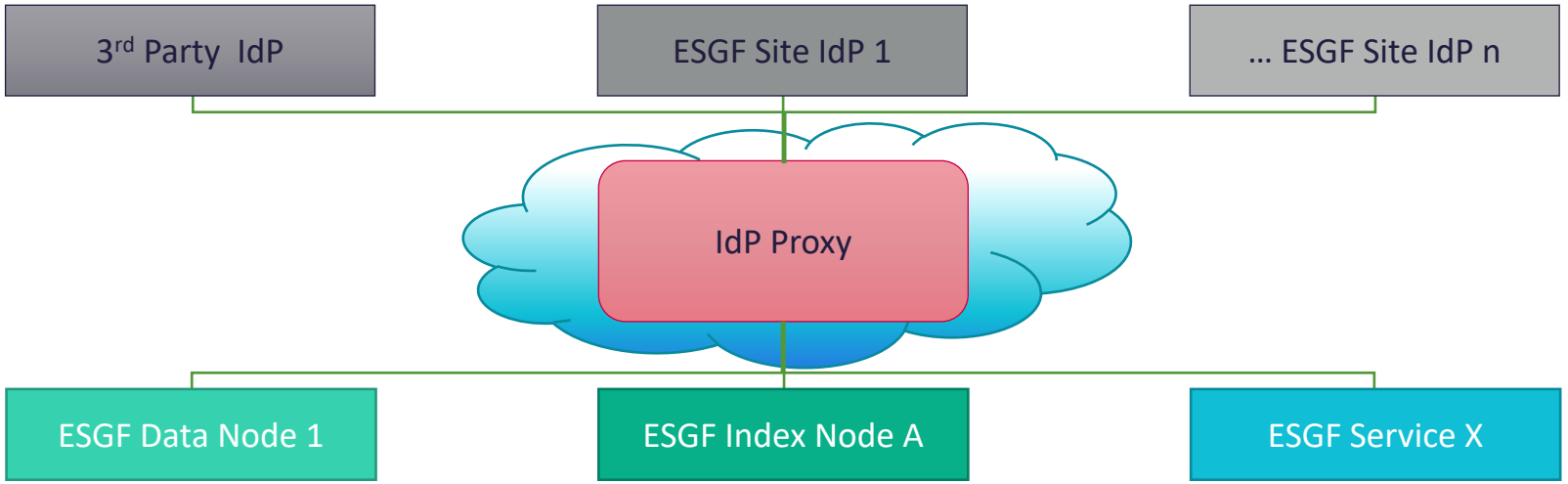
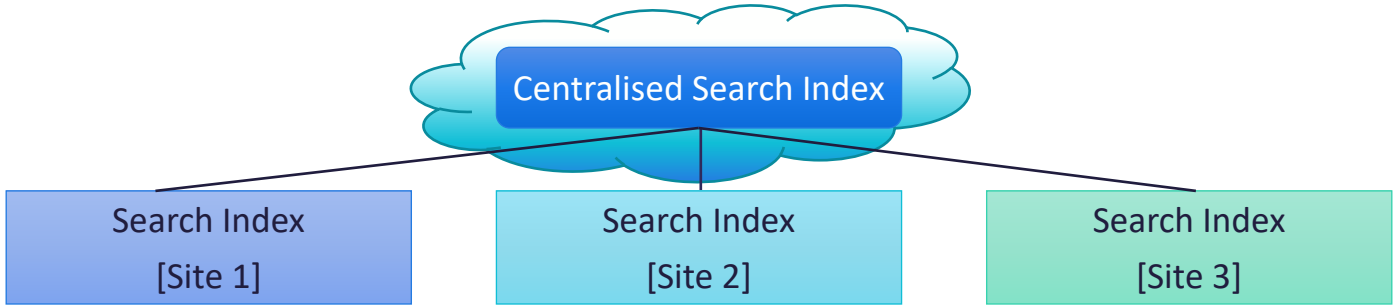
Cloud and Identity Management

- Existing status quo: Many-to-many relationships: too complicated
- AARC Blueprint: Identity Proxy - Acts as abstraction between ESGF services and IdPs



Cloud and Search: Centralised Search Index



- Centralised cloud-hosted search index harvests content from all providers
- Builds on existing technology in ESGF (Apache Solr) but reduces operational burden for hosting sites and provides a single-entry point for users

Cloud and data access and storage

Opportunities

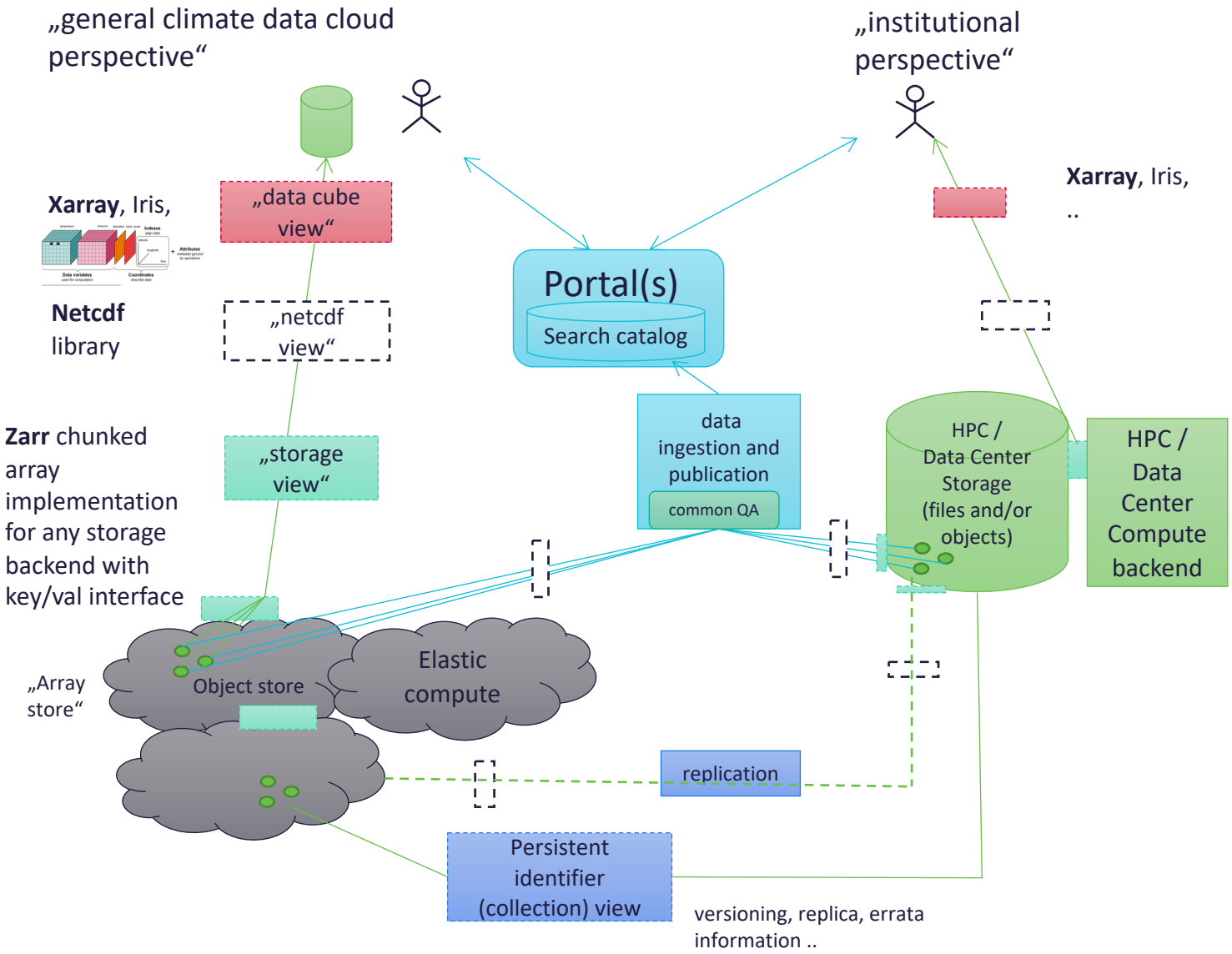
- New paradigms for massively parallel data storage and access, such as object store
  - Xarray and zarr
- Potential point of entry for scientists without access to large-scale computing, analysis, and network resources

Challenges

- Public cloud not cost effective for *long-term, large-scale* data storage and access
- Most on-premise data centres still have POSIX file systems (Though some are experimenting with object store – JASMIN)
- Concerns about Xarray/zarr for data archiving – consistency, integrity and metadata retention

Cloud vs. institutional Perspective

(Diagram courtesy of Stephan Kindermann, DKRZ)



Role of standards

- Critical for hosting centres in ESGF
  - These increasingly support a broader range of domains and communities in the Earth sciences.
  - Interoperability with other similar systems, minimise duplication and maximise re-use

- Data
  - CF-netCDF continues as established standard for this community
  - Challenges around storage and access with Xarray and zarr: how to maintain data integrity and consistency
  - New standards evolving – with end-user centric perspective e.g. https://portal.ogc.org/files/?artifact_id=91644#PartDAPA

- Identity management
  - Adopt standards and use off-the-shelf solutions where possible - OIDC (OpenID Connect) and Keycloak

- Search – ESGF uses its own standard based on Apache Solr API, these standards are being explored as alternatives:
  - OpenSearch (http://ceos.org/ourwork/workinggroups/wgiss/access/opensearch/)
  - STAC (https://stacspec.org)
  - ESM Collection Specification (https://github.com/NCAR/esm-collection-spec)

Conclusions and next steps

- Cloud enables major architectural changes to be made to simplify
  - Centralised search and identity services

- Storage and data access is at a cross-roads:
  - POSIX access continues to dominate for on-premise
  - Object storage on cloud provides new possibilities
  - No community-wide consensus on a single solution yet

- A roadmap for re-development of ESGF has been established
  - Incremental releases with initial new baseline version ready for the summer

Thank you

- This work has been carried out through IS-ENES3, a project funded by the European Union's Horizon 2020 research and innovation programme under grant agreement No 824084

- Free access to computing platforms for multi-model climate data analyses for CMIP6 and CORDEX ! –
  - https://portal.enes.org/data/data-metadata-service/analysis-platforms

- More information at EGU sessions …
  - CL5.7 Climate Services – Underpinning, 05 May, 10:45–12:30, EGU 2020-19121: https://meetingorganizer.copernicus.org/EGU2020/session/36737
  - CL2.6 Detecting and attributing climate change: trends, extreme events, and impacts, 07 May, 08:30–10:15, EGU 2020-19340: https://meetingorganizer.copernicus.org/EGU2020/session/36768