

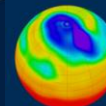


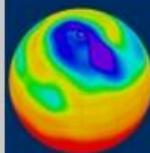
JASMIN, Common Data Issues and more...

Numerical Simulations at scale are all about
logistics!

November 25, 2015

Ag Stephens and Bryan Lawrence
(STFC Centre for Environmental Data Analysis)





Centre for Environmental Data Analysis

SCIENCE AND TECHNOLOGY FACILITIES COUNCIL
NATURAL ENVIRONMENT RESEARCH COUNCIL



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Welcome to the Centre for Environmental Data Analysis

The Centre for Environmental Data Analysis (CEDA) serves the environmental science community through **four data centres**, **data analysis environments**, and participation in a host of relevant research **projects**.

We aim to support environmental science, further environmental data archival practices, and develop and deploy new technologies to enhance access to data. Additionally we provide services to aid large scale data analysis.

You can learn more about our data centres, our data processing services, and project work using the links in the menu above.

If you have a particular project or data management issue that you would like to consult CEDA on please **contact** us and a member of the **CEDA team** will be happy to assist.

CEDA News

Recent News

- [CEDA Web Processing Service \(CEDA WPS\) back up](#) July 14, 2015, 5:29 p.m.
- [Dataset Showcase: CRU Climate Data](#) June 25, 2015, 8:56 a.m.
- [CEDA ESGF nodes unavailable](#) June 17, 2015, 12:37 p.m.



National Centre for
Atmospheric Science

[Accessibility](#) [Disclaimer](#) [Privacy and Cookies](#)



National Centre for
Earth Observation

NATURAL ENVIRONMENT RESEARCH COUNCIL



Our data centres

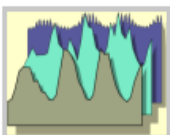
Data Centres

The Centre for Environmental Data Archival is responsible for the running of the following data centres:



The British Atmospheric Data Centre

The British Atmospheric Data Centre (BADC), NERC's designated data centre for the UK atmospheric science community, covering climate, composition, observations and NWP data.



The UK Solar System Data Centre

The UK Solar System Data Centre, co-funded by STFC and NERC, curates and provides access to archives of data from the upper atmosphere, ionosphere and Earth's solar environment.



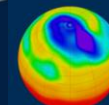
NERC Earth Observation Data Centre

The NEODC is NERC's designated data centre for Earth Observation data and is part of NERC's National Centre for Earth Observation.



IPCC Data Distribution Centre

The Intergovernmental Panel on Climate Change (IPCC) DDC provides climate, socio-economic and environmental data, both from the past and also in scenarios projected into the future. Technical guidelines on the selection and use of different types of data and scenarios in research and assessment are also provided. UK Climate Projections.



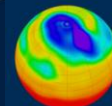


Outline

- JASMIN
- Common data issues
- Big data and scale
- Where to put the data?
- ESGF
- Constraints and how they influence what we can do



JASMIN - what is it?





A platform for data processing

Storage

- **15 PB high-performance disk storage:**
 - CEDA archive (5 PB)
 - Over 100 Group Workspaces for projects/groups (10PB).
- Equivalent capacity in near-line **tape** system

Compute

- ~4000 compute nodes, interchangeably deployable in either:
 - batch compute cluster (**LOTUS**), or
 - cloud hosting environment
- Individual scientific analysis servers





<http://www.jasmin.ac.uk>

JASMIN

What is JASMIN ▾

Services ▾

Users ▾

Get Access ▾

How to Use ▾

Help ▾

FAQ

Search

Go

Petascade storage and cloud computing for big data challenges in environmental science

[Learn more »](#)

Data-intensive computing

JASMIN provides the UK and European climate and earth-system science communities with an efficient data analysis environment. Many datasets, particularly model data, are too big to be easily shipped around: JASMIN enables scientists to bring their processing to the data.

Flexible data access

JASMIN provides new ways for scientists to collaborate in self-managing group workspaces, enabling models and algorithms to be evaluated alongside curated archive data, and for data to be shared and evaluated before being deposited in the permanent archive.

Scalable future

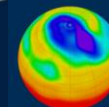
JASMIN enables [CEDA](#) to carry out its mission of data curation and facilitation more efficiently. Fast, parallel, scalable storage provides a home for in-demand archive data, while a virtualised server infrastructure provides a more capable base for delivery of CEDA's data centre services to the science community.





A quick tour of JASMIN

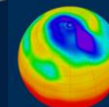
- Services: Overview diagram, GWS, JAP, LOTUS, HPDT
- Users: brief
- Get Access: signing up, managing SSH keys, IP reg, Login
- How to Use: navigate - and others.
- Help: contact us





JASMIN analysis servers (open to all)

| Server | CPUs | Memory |
|--------------------------------|-----------|------------|
| jasmin-sci1.ceda.ac.uk | 8 | 32Gb |
| jasmin-sci2.ceda.ac.uk | 8 | 32Gb |
| jasmin-sci3.ceda.ac.uk | 48 | 2Tb |
| cems-sci1.cems.rl.ac.uk | 8 | 16Gb |
| cems-sci2.cems.rl.ac.uk | 48 | 2Tb |



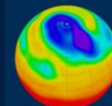
JASMIN Analysis Platform (JAP)

- Software stack for scientific analysis on JASMIN (and elsewhere)
- Common packages for climate science and geospatial analysis
- O/S: RHEL6, CentOS6.
- Deployed on JASMIN
 - Common "Science" servers
 - LOTUS
 - Sci Virtual Machine "template"





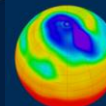
Common data issues





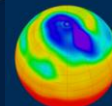
Standards - how they help/hinder us

- CMOR, CF-netCDF, ISO19115, DRS etc...
- They clearly have great value:
 - CMIP5 demonstrated how such efforts could have significant benefits
 - E.g. "everyone called tas 'tas' and rcp45 'rcp45'"
- And they have great cost:
 - CMIP5 demonstrated that we could expend a lot of effort agreeing standards
 - And a lot more effort trying to implement them
- Do we have a choice?
 - Without standards we'll get nowhere
 - But we need to **communicate** the standards are and **provide tools to help people comply**.





Example Tasks and Deliverables in PRIMAVERA and CRESCENDO





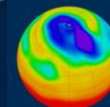
Data Management Plans

Within PRIMAVERA we will produce and implement the Data Management Plan (DMP) as part of participation in the Open Research Data Pilot.

DMPs are useful for:

- Making us plan for data issues
- Communicating the lifecycle of different data within a project:
 - Third-party data used
 - Data generated
 - Formats, metadata, longevity, storage etc.
 - Final dissemination

They work best as living documents!





Example tasks

PRIMAVERA Data Specification:

- The specification of the Required Inputs and Outputs is a prerequisite for all Stream 1 simulations in WP6, based on CMIP5.

PRIMAVERA Data Conversion:

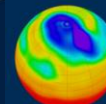
- Establish the methodology and workflow for bringing data to JASMIN and **converting to the standard data format specified** in the DMP.

Both projects: Publishing to ESGF

- Making key data sets available via ESGF interfaces.

CRESCENDO: Improvements to ESMValTool

- Common code to validate model outputs (including comparison with other data) - *code near the data*





Colocation with other data

- "Bring the code to the data" - is a useful approach when working with climate simulations.
- An advantage of platforms like JASMIN is that your project data is available alongside existing archived, and current project, data sets such as:
 - CMIP5
 - CORDEX
 - ERA-Interim

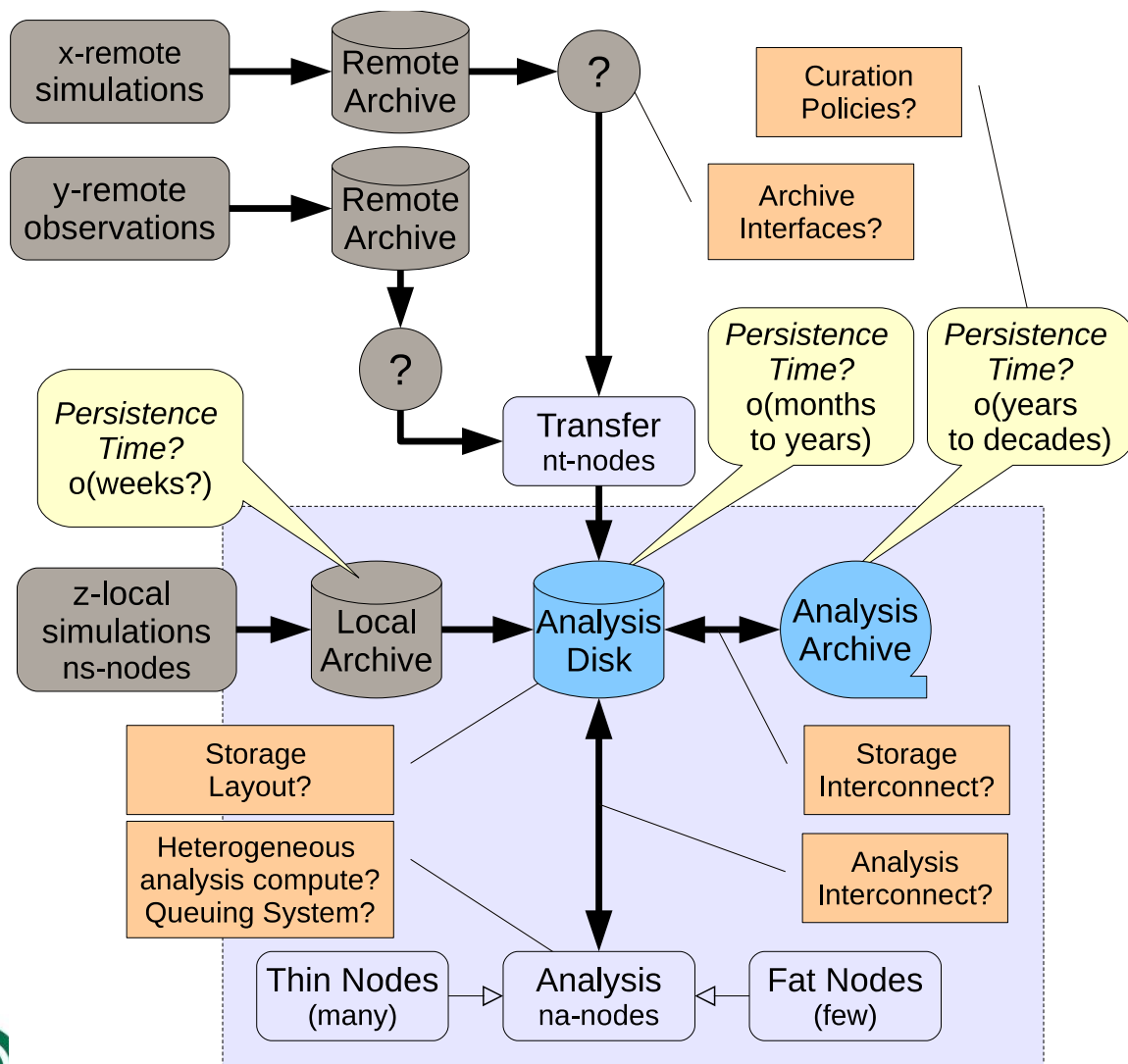
Hence our JASMIN Analysis Platform

But what if you need other codes?





Common project elements (PRIMAVERA, CRESCENDO and beyond)



In both projects we have **remote simulations** in many places.

In both projects we want a **common analysis environment** and **downstream services**.

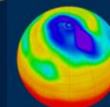
In both projects we have to deal with **differing persistence of differing data**.



Quality checking

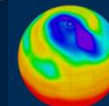
There are different levels of quality checking that we need to be clear about:

1. The Scientist runs his/her own quality assurance on the simulations to check the **scientific integrity** of the results.
2. The Data Manager runs his/her **compliance checks** on the data files to ensure that the metadata, file-naming and data structures meet **an agreed common specification**.
3. What is *intrinsic* data quality (that the data producer worries about) and what is *extrinsic* data quality (that the end-user is concerned with)?



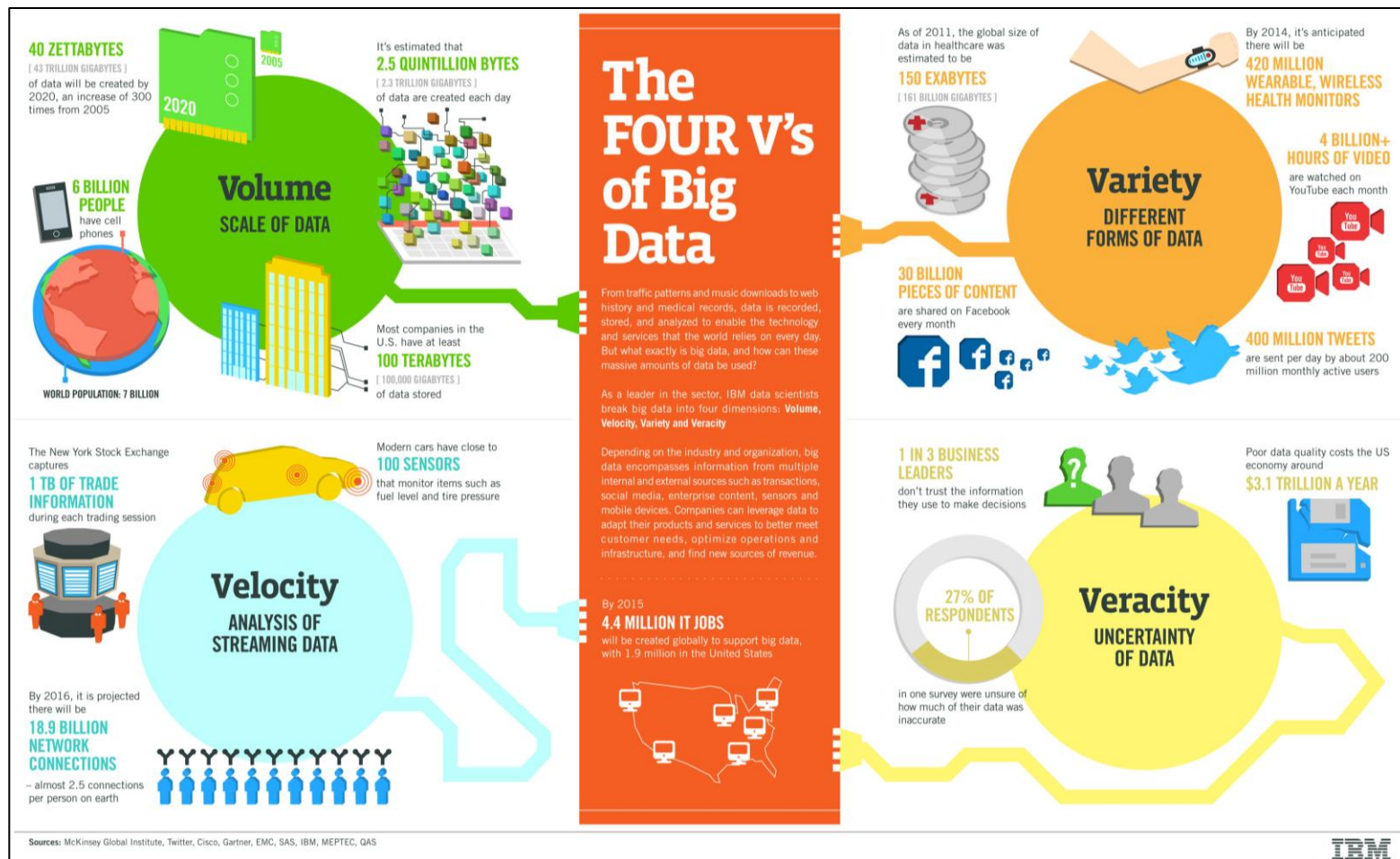


The problem with extrinsic quality

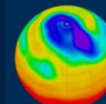




Is climate data "Big Data"?



IBM





Thinking about scale (CMIP5)

Fifth Climate Model Intercomparison Project (CMIP5)

World Climate
Research
Programme
WCRP- WGCM
*Production involved all
the major climate
modelling centres*

Original Timing:

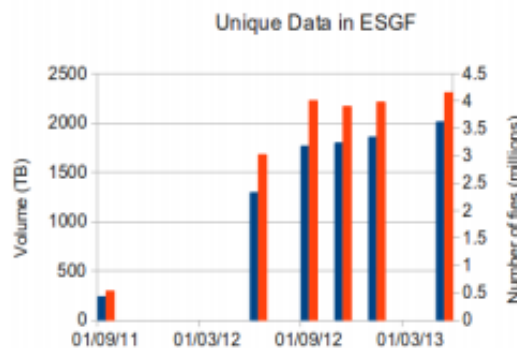
- Expect $o(2)$ PB of requested output from 20+ modelling centres finished early 2010!

Actual Timing?

- Years late.

(23/05/13):

101 experiments
61 model variants
590,000 datasets!
4.5 million files
2 PB in global archive
Unknown PB locally!



Blue: Volume; Red: Files

(NB: replicas and versions!)

Data Delivered by:

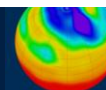
PCMDI-led, community
developed (GO-ESSP)
s/w infrastructure for
data delivery:

**Earth System Grid
Federation (ESGF)**



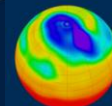
And now we have to deal with this!

| | Short name of MIP | Long name of MIP |
|----|--------------------|---|
| 1 | AerChemMIP | Aerosols and Chemistry Model Intercomparison Project |
| 2 | C4MIP | Coupled Climate Carbon Cycle Model Intercomparison Project |
| 3 | CFMIP | Cloud Feedback Model Intercomparison Project |
| 4 | DAMIP | Detection and Attribution Model Intercomparison Project |
| 5 | DCPP | Decadal Climate Prediction Project |
| 6 | FAFMIP | Flux-Anomaly-Forced Model Intercomparison Project |
| 7 | GeoMIP | Geoengineering Model Intercomparison Project |
| 8 | GMMIP | Global Monsoons Model Intercomparison Project |
| 9 | HighResMIP | High Resolution Model Intercomparison Project |
| 10 | ISMIP6 | Ice Sheet Model Intercomparison Project for CMIP6 |
| 11 | LS3MIP | Land Surface, Snow and Soil Moisture |
| 12 | LUMIP | Land-Use Model Intercomparison Project |
| 13 | OMIP | Ocean Model Intercomparison Project |
| 14 | PMIP | Palaeoclimate Modelling Intercomparison Project |
| 15 | RFMIP | Radiative Forcing Model Intercomparison Project |
| 16 | ScenarioMIP | Scenario Model Intercomparison Project |
| 17 | VolMIP | Volcanic Forcings Model Intercomparison Project |
| 18 | CORDEX* | Coordinated Regional Climate Downscaling Experiment |
| 19 | DynVar* | Dynamics and Variability of the Stratosphere-Troposphere System |
| 20 | SIMIP* | Sea-Ice Model Intercomparison Project |
| 21 | VIACS AB* | VIACS Advisory Board for CMIP6 |





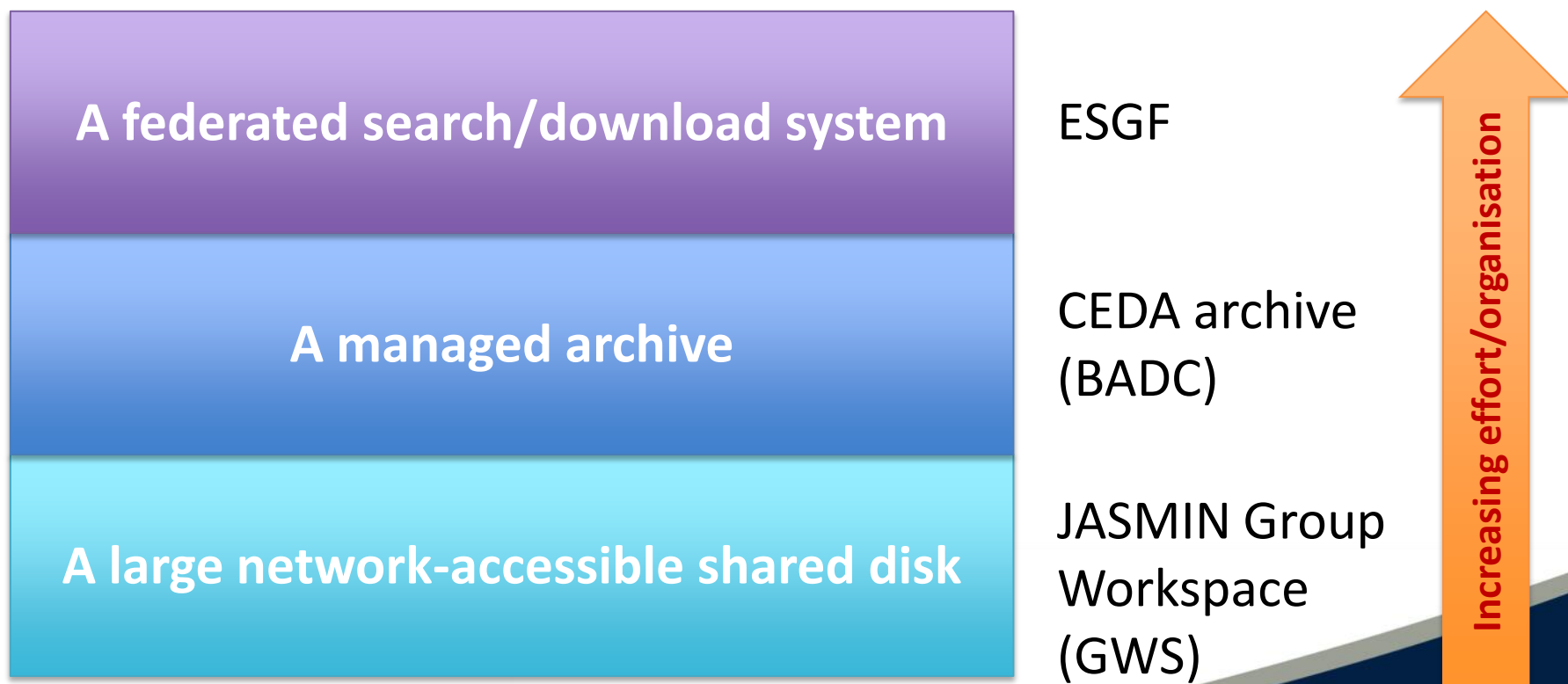
Where to put data?





ESGF is not the right answer to every question

We can answer the "where can I put my simulations?" question in three layers:





It all depends what you need to do

Who do you want to share with?

- Small group of collaborators → GWS
- The world → Archive and/or ESGF

How visible do you want to data to be?

- Partially - through SSH or simple web file list → GWS
- Visible through some catalogues/discovery systems → Archive
- Visible alongside high-profile climate projects/datasets → ESGF

How long should your data persist?

- Months to a few years → GWS
- Longer → Archive and/or ESGF - **which will live longer?**

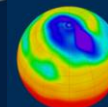


What can a GWS offer?

- For “projects” that want to:
 - Share a LARGE network-accessible disk.
 - Allow access from a number of institutions.
 - Pull data from external sites to a common cache.
 - Push data to external sites.
 - Process/analyse the data (on batch compute).
 - Process/analyse the data in conjunction with other *archived* or *group workspace* datasets.

A large network-accessible shared disk

JASMIN Group
Workspace
(GWS)





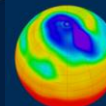
Danger of "useful" shared disk solution

The problem with providing an effective shared disk approach (GWS) is the data providers can think:

"My data is on CEDA = Job done!"

"This is much easier than spending days/weeks producing metadata and documenting my method."

But data will NOT persist here!





A managed archive (e.g. CEDA)

- Agree formats and metadata
- High level metadata records: Project, people, collection, model, computation, instrument, platform etc.
- Data managers involved in ingestion process - *at least now!*

A managed archive

CEDA archive
(BADC)



Data Catalogue (metadata)

<http://catalogue.ceda.ac.uk>

The screenshot displays the CEDA Data Catalogue interface. The header includes the CEDA logo, navigation links (Contact us, CEDA Help, News), and a search bar. The main content area shows search results for the project "NCAS mobile X-band radar scan data from Davidstow Airfield during the MICROphysics of CONvective PRecipitation (MICROSCOPE) project". The project description states that the data was collected at the Davidstow Airfield, Cornwall, between June and August 2013 as part of the MICROSCOPE project. The X-band radar is operated as part of the NCAS Atmospheric Measurement Facility's (AMF). The project is cited as: Bennett, L. (2015): NCAS mobile X-band radar scan data from Davidstow Airfield during the MICROphysics of CONvective PRecipitation (MICROSCOPE) project. NCAS British Atmospheric Data Centre, date of citation. <http://catalogue.ceda.ac.uk/uuid/4bb383b7d6ca421bbdd57b8097d5664>. The keywords listed are: COPE, radar, precipitation, rainfall, dual-polarisation, Doppler, clouds, microphysics, clear-air echoes, convection, storms, dynamics, rainfall. The project is part of the Dataset Collection: MICROphysics of CONvective PRecipitation (MICROSCOPE) project. The previous info section indicates no news update for this record. The temporal range is from 2013-07-18T00:00:00 to 2013-08-17T23:59:59. The geographic extent is shown on a map of the United Kingdom, with a red box indicating the location of the Davidstow Airfield. The map data is from 2015 Google.

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Find data related to Input search term... in Datasets GO!

Catalogue Home Catalogue Intro Advanced Search Admin login

NCAS mobile X-band radar scan data from Davidstow Airfield during the MICROphysics of CONvective PRecipitation (MICROSCOPE) project

Dataset
Update Frequency: Not Planned
Status: Completed
Publication State: Published
Publication Date: 2015-03-10
[Edit Record (Admin only)]

Abstract
Scan data from the National Centre for Atmospheric Science's (NCAS) mobile X-band radar collected at the Davidstow Airfield, Cornwall, between June and August 2013 as part of the MICROphysics of CONvective PRecipitation (MICROSCOPE) project. The X-band radar is operated as part of the NCAS Atmospheric Measurement Facility's (AMF).

Citable as: Bennett, L. (2015): NCAS mobile X-band radar scan data from Davidstow Airfield during the MICROphysics of CONvective PRecipitation (MICROSCOPE) project. NCAS British Atmospheric Data Centre, date of citation. <http://catalogue.ceda.ac.uk/uuid/4bb383b7d6ca421bbdd57b8097d5664>

Keywords: COPE, radar, precipitation, rainfall, dual-polarisation, Doppler, clouds, microphysics, clear-air echoes, convection, storms, dynamics, rainfall

Temporal Range
2013-07-18T00:00:00 2013-08-17T23:59:59

Geographic Extent
Map of the United Kingdom showing the location of the Davidstow Airfield (red box). Map data ©2015 Google.

Details Process Variables Linked Documentation (1)

Project: The NERC MICROphysics of CONvective PRecipitation (MICROSCOPE) project as part of the CONvective PRecipitation Experiment (COPE)

Dataset is part of: Dataset Collection: MICROphysics of CONvective PRecipitation (MICROSCOPE) pro...

Previous Info: No news update for this record

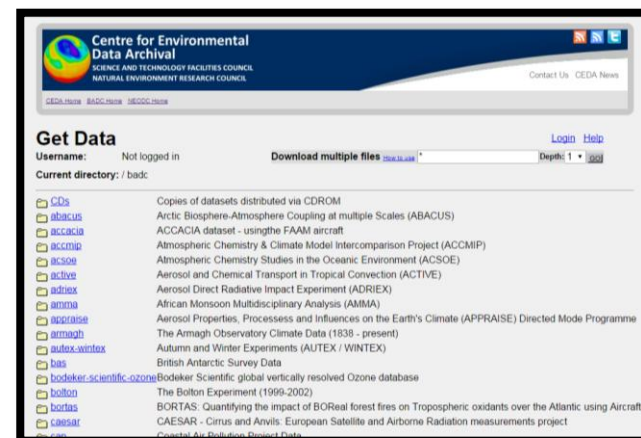
DOI can be assigned at this level



Data Access Tools

Generic services:

- HTTP-based "**Browse**" service →
- **FTP** access
- **OpenDap** service now launched: <http://dap.ceda.ac.uk>





Publishing to ESGF

A federated search/download system

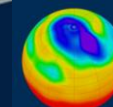
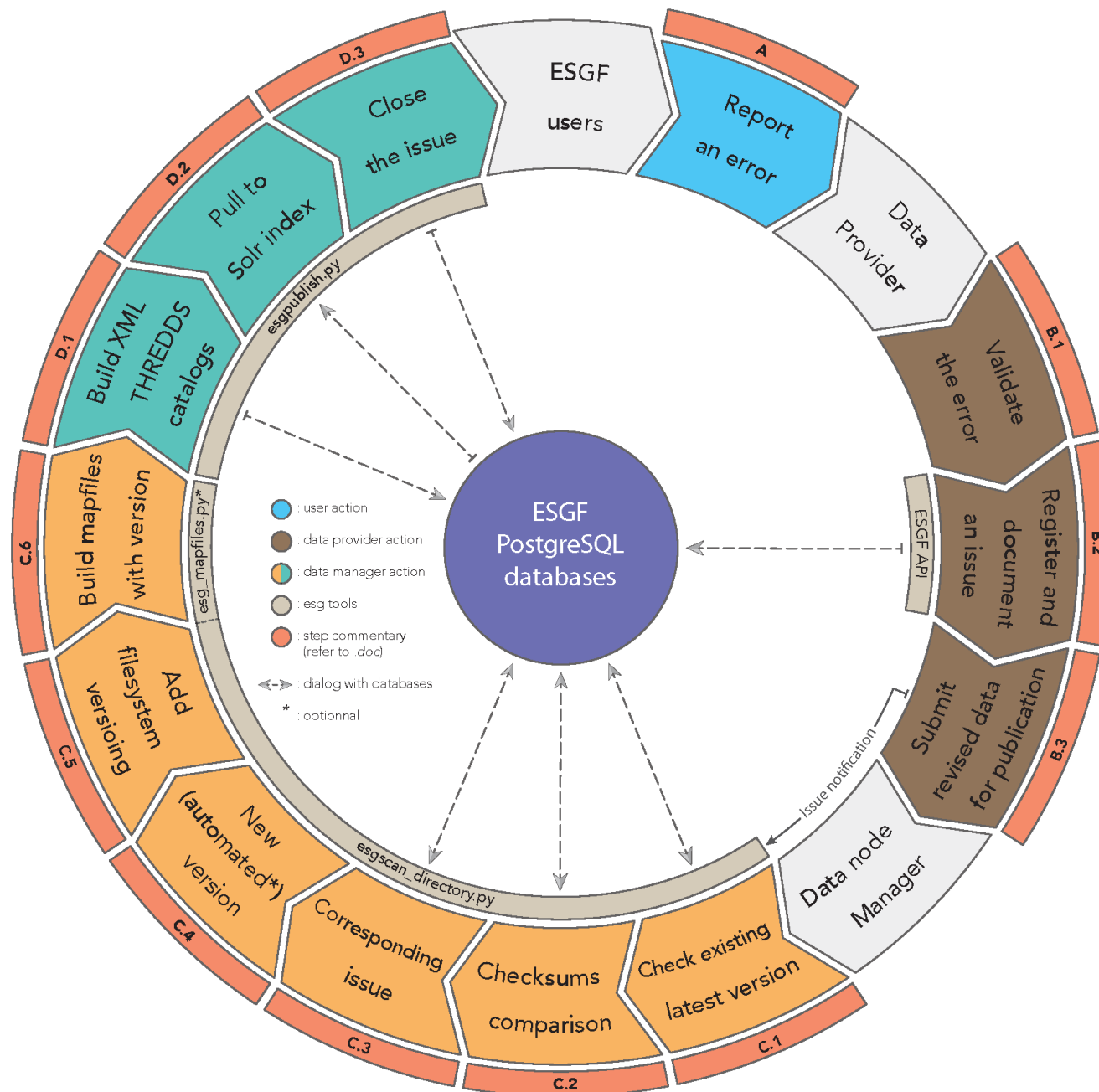
ESGF

The MIP "Data Workflow"

(courtesy of Guillaume
Levavasseur - IPSL)

We are working closely
with ESGF partners.

Automation
is essential





ESGF (through a browser)



HomeSearchToolsLoginHelp

Current Selections

- [remove all](#)
- [\(x\) model:HadGEM2-ES](#)
- [\(x\) data node:esgf-data2.ceda.ac.uk](#)
- [\(x\) product:output1](#)
- [\(x\) time frequency:6hr](#)
- [\(x\) realm:atmos](#)
- [\(x\) ensemble:r2i1p1](#)
- [\(x\) experiment:historical](#)

Search Categories

| |
|-------------------|
| Project |
| Institute |
| Model |
| Instrument |
| Experiment Family |
| Experiment |
| Time Frequency |

Examples: *temperature*, *"surface temperature"*, *climate AND project:CMIP5 AND variable:hus*.
To download data: add datasets to your Data Cart, then click on *Expand* or *wget*.

☒ Search All Sites ☒ Show All Replicas ☐ Show All Versions

< 1 > displaying 1 to 2 of 2 search results

Display datasets per page

[Add All Displayed to Datacart](#) [Remove All Displayed from Datacart](#)

ResultsData Cart

project=CMIP5 / IPCC Fifth Assessment Report, model=HadGEM2-ES, Met Office Hadley Centre, experiment=historical, time_frequency=6hr, modeling realm=atmos, ensemble=r2i1p1, version=20130418
Data Node: [esgf-data2.ceda.ac.uk](#)
Version: 20130418
Description: HadGEM2-ES model output prepared for CMIP5 historical
Further options: [Add To Cart](#) [Model Documentation](#)

project=CMIP5 / IPCC Fifth Assessment Report, model=HadGEM2-ES, Met Office Hadley Centre, experiment=historical, time_frequency=6hr, modeling realm=atmos, ensemble=r2i1p1, version=20130419
Data Node: [esgf-data2.ceda.ac.uk](#)

[Temporal Search](#)
[Clear search](#)
[constraints and datacart](#)
[Search Help](#)
[Search Controlled](#)
[Vocabulary](#)

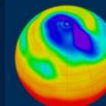
Environmental

SCIENCE & TECHNOLOGY FACILITIES COUNCIL
RCH COUNCIL



ESGF is NOT funded!

- No single project is paying the real costs of their storage, for the physical disk/tape media, or for the people involved. Not even the true cost of the people to do the massaging ...
- The entire ediface depends on the careful construction of infrastructure that can be built from **contributions of many different projects** for many different audiences:
 - Hardware, Software, Metadata
 - Tools and utilities
 - No one project has control over any of those things:
 - **Not even WGCM/CMIP.**
 - **Not Primavera and Crescendo.**





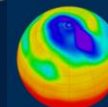
Versioning

CMIP5 made great advances in the management of versioning:

- Multiple data set versions can be made documented and accessible side-by-side
- Preserves provenance
- Follows good curation principles

Within CMIP5, versioning was managed **inconsistently across the federation**, resulting in:

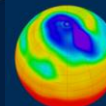
- Inability to determine whether data has changed (on server)
- Different nomenclature at different sites ("v1" vs "v20110424")





The impact of Petascale

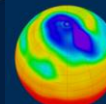
Both PRIMavera and CRESCENDO will produce
large volumes of data.





Too much data, not enough disk

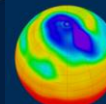
- Hitting Petascale has implications...
- The cost of (high-performance) disk continues to be significantly higher than tape.
- At CEDA, we have survived a long time with a disk-based solution.
- At this scale we need a tape-based solution with caching of "popular" data - *currently under development*.
- **This becomes relevant to all projects delivering big data!**
- We may ask:
 - What is the most important data (that should stay in the cache)?





Too many users, not enough compute - A word or two about compute platforms

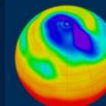
- Our 4,000 core LOTUS cluster (on JASMIN) has been a game-changer for some scientists analysis/inter-comparing data.
- However, with capability comes new requirements ...
- How can we continue to deliver compute power as demand grows? Do we need a focussed solution?





The wrong compute?

- "Bring the compute to the data" has been our mantra for the last couple of years.
- But sometimes it's "your compute" not mine. How can we enable seamless shipping of code between different physical environments.
- The next phase is multiple deployment environments
 - **Batch clusters** - already in place
 - **Scaling containers** (e.g. using Docker) in the future.
- IaaS (Infrastructure as a Service) versus PaaS (Platform as a Service) in the (local/private) Cloud.





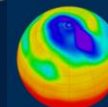
Coming back to MIPs

Model Intercomparison Projects are a response to two factors:

1. The need to evaluate our assumptions and our models. Evaluation requires comparison, and differing ways of doing simulation.
2. The need to share information between groups. Organising and delivering this at scale is hard.

All of this is bigger than any one group can do alone. In the UK, the response has been the UKESM programme, bringing many more communities into the ESM frame.

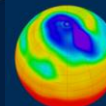
As move to more societally relevant science (the “grand challenge”), we will have more and **more communities in play, and more evaluation to do.**





Scale, Information, Collaboration and MIPs

- Both the computing and the human trends are towards scale!
- At scale, we need to formally codify information.
- Dealing with the volume, variety, and velocity of data, being shared by multiple communities, requires more than just unstructured documents to capture information and requirements. **Need metadata (targeted at specific parts of workflow), controlled vocabularies, tools and automation.**
- There is a necessary inertia in developing, populating, and exploiting information systems at scale. Agility, at scale, is hard!
- We all need to get used to “**conforming**” if we want to collaborate, and future MIPs are going to require even more information constraints, from definitions, to data outputs.

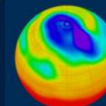




Effective data management at scale

What can/do we do to manage data at scale?

- Employ standards and conventions:
 - Our catalogue is based on ISO standards for describing environmental science data and geospatial information...
 - ...but we need to adapt it to our communities' needs.
- Employ consistent methods of naming (e.g. using common vocabularies) and describing data.
- Promote decent data formats (for re-usability and tool development)...
 - I.e. NetCDF and the CF Metadata Conventions





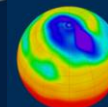
We need more Data Managers (inside projects)

Given this situation:

- ~~The only way forward is to employ 100s more Data Managers at Data Centres.~~

unlikely

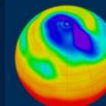
- The only way forward is for data providers to become more active in the data management:
 - Organising/communicating data standards and specifications
 - Actively available disk/tape allocation
 - Establishing methods of data reduction (e.g. reducing precision or sub-setting)
 - Migrating to tape to free up space.





Conclusions

- PRIMavera and CRESCENDO are projects that contribute to and exploit the “CMIP era”:
 - They will generate data that will be “available in ESGF”
 - The project teams will be analysing their (big) data
 - Downstream users will include
 - Expert users of modelling data
 - Novice users of modelling data
- There is a long way between the HPC platform where the data is generated and the data appearing in ESGF.
 - Not all data should travel that route.
 - Most data will need massaging to make it all the way.





Conclusions

Everything is scaling up: number of experiments, models, projects, files, size of files, requirements for post-processing etc.

- Data Management facilities are also scaling (which buys us time)...
- ...but the Data Managers are not multiplying.

So we need to evolve:

- Automate everything!
- Engage the scientists to:
 - Prepare data/metadata according to agreed standards
 - Become part of the data management process