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CMIP, CSSEF, ESGF, and BER Related Data Projects: Climate Model Analysis, Visualization, and Test Bed Efforts for Ultra-Large Data Sets

Dean N. Williams and Dave Bader on behalf of Multiple Earth System Communities and Projects

Federated and Integrated Data from Multiple Sources

CESD Data Meeting – Infrastructure and Framework Presentation ◆ June 26, 2012

Outline

- CMIP5 – Redefined requirements for data federation
- ESGF concept
- ESGF and CMIP
- ESGF pilot projects with ARM and CDIAC
- CSSEF
- Associated BER efforts
- Current status and near term directions
- A possible long-term vision for BER's "Climate K-Base"

CMIP: Experiment Design

CMIP5: 47 models available from 21 centers

- CMIP = **Coupled Model Intercomparison Project**
  - Phase 1: Idealized simulations of present-day climate
  - Phase 2: Idealized simulations of future climate changes
  - Phase 3: More realistic simulations (2004 – present)
- **CMIP 5** multi-model archive expected to include
  - **3** suites of experiments
  - **24** modeling centers in **19** countries
  - **58** models
  - Total data, **~3.5 PB**
  - Replica **1 – 2 PB**
  - Derived data **~1 PB**
- **Global distribution**
- **Timeline fixed** by IPCC (2012 - 2013)
- **LLNL organizes, manages and distributes** the CMIP/IPCC (Intergovernmental Panel on Climate Change) database of climate model output

CMIP3 archive vs. CMIP5 archive

CMIP3 Modeling Centers		volume (GB)
NCAR	USA	9,173
MIROC3	Japan	3,975
GFDL	USA	3,843
IAP	China	2,868
MPI	Germany	2,700
CSIRO	Australia	2,088
CCCma	Canada	2,071
INGV	Italy	1,472
GISS	USA	1,097
MRI	Japan	1,025
CNRM	France	999
IPSL	France	998
UKMO	UK	973
BCCR	Norway	862
MIUB	Germany/Korea	477
INMCM3	Russia	368
Totals		**34,989 (TB)**

35 TB

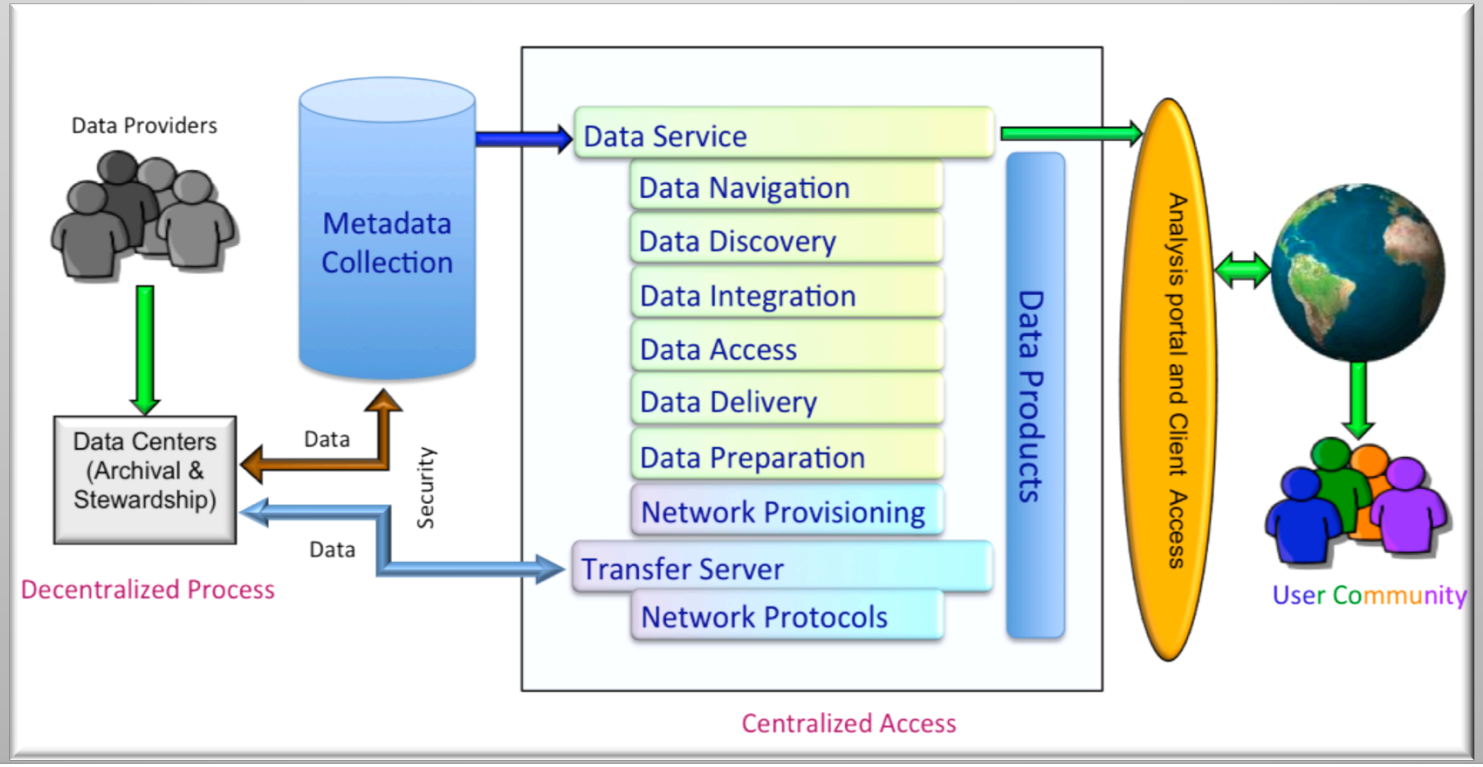
CMIP5 Modeling Centers		volume (TB)
BCC	China	51
CCCma	Canada	51
CMCC	Europe (Italy)	158
CNRM	France	71
CSIRO	Australia	81
EC-EARTH	Europe (Netherland)	97
GCESS	China	24
INM	Russia	30
IPSL	France	121
LASG	China	100
MIROC	Japan	350
MOHC	UK	195
MPI	Germany	166
MRI	Japan	269
NASA	USA	375
NCAR	USA	739
NCC	Norway	32
NCEP	USA	26
NIMR/KMA	Korea	14
NOAA GFDL	USA	158
Totals		**3,108 (PB)**

3.1 PB
Currently 1.2 PB

CMIP5/CMIP3 = 10^2

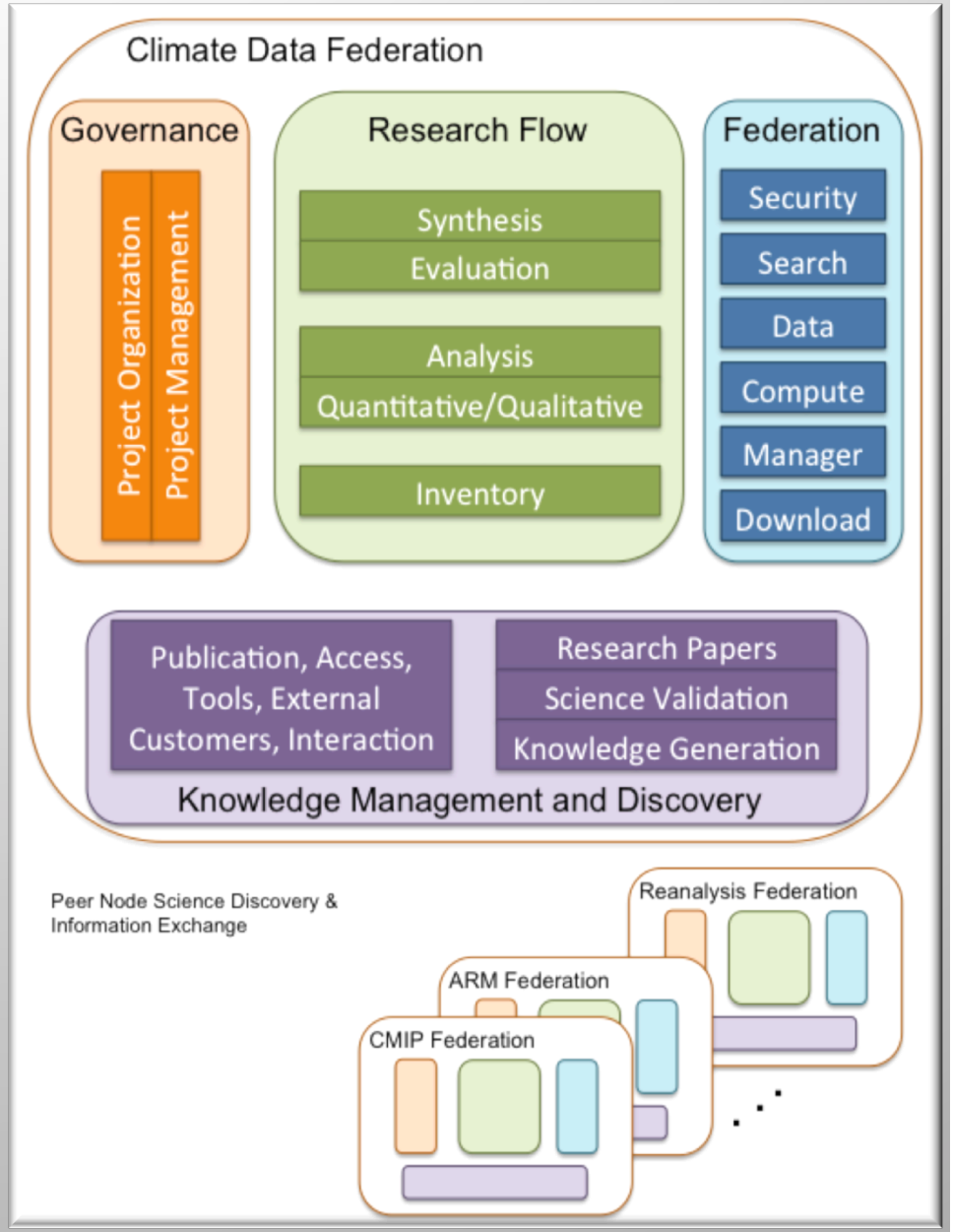
Big Data Challenges

- **Centralized process** for CMIP3, data was shipped to LLNL via disk, then made available to users
  - Several weeks delay between generation of files and availability to users
  - Correction errors in data was too difficult
  - LLNL became a single point of failure (a catastrophic crash of our RAID system meant data was inaccessible for several weeks)
  - Backup was incredibly difficult, which made restoration equally as hard
- **Decentralized process** for CMIP5, a new (and more complicated approach) was necessary
  - Distributed data Archive
  - No single point of failure
  - Replication of heavily-used data sets
  - Data can be made available without delay and can be corrected locally



Data Federation Services

- NetCDF Climate and Forecast (CF) Metadata Convention
  - (LibCF)
  - Mosaic
- Climate Model Output Rewriter 2 (CMOR-2)
- GRIDSPEC & SCRIP
- Publishing
- Search & Discovery
- Replication and Transport
  - GridFTP, OPeNDAP, DML, Globus Online, ftp, BeSTMan (HPSS)
  - Networks
- Data Reference Syntax (DRS)
- Common Information Model (CIM)
- Quality Control
  - QC Level 1, QC Level 2, QC Level 3, Digital Object Identifiers (DOIs)
- Websites and Web Portal Development
  - Data, Metadata, Journal Publication Application
- Notifications, Monitoring, Metrics
- Product Services
  - Live Access Server, UV-CDAT
- Security



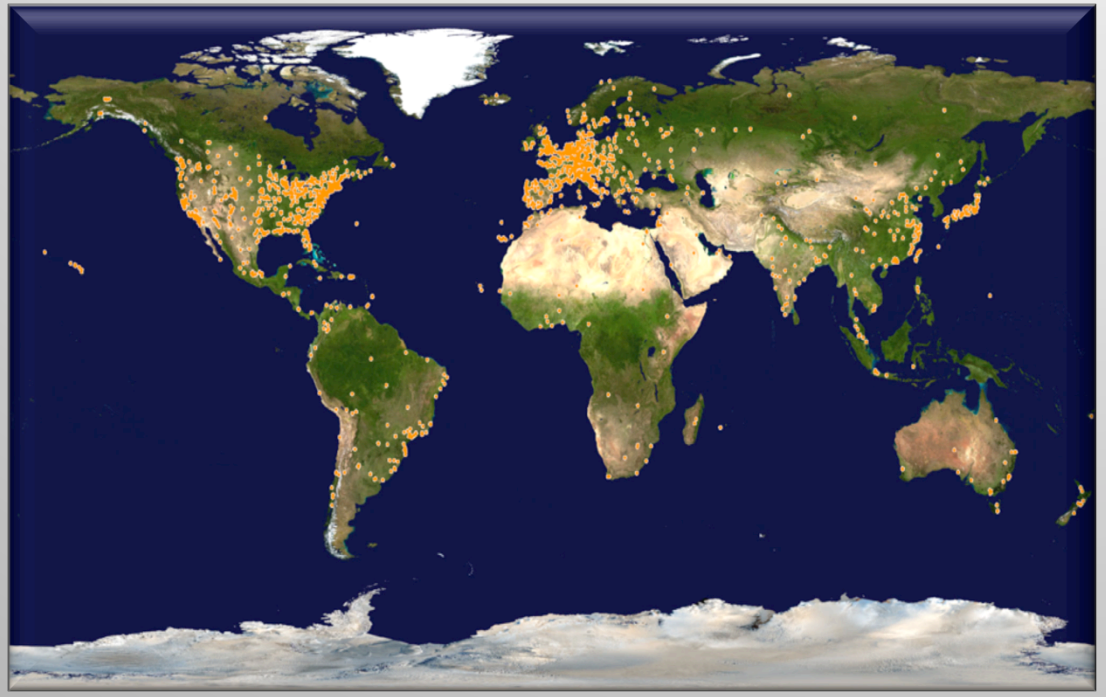
Earth System Grid Federation (ESGF)

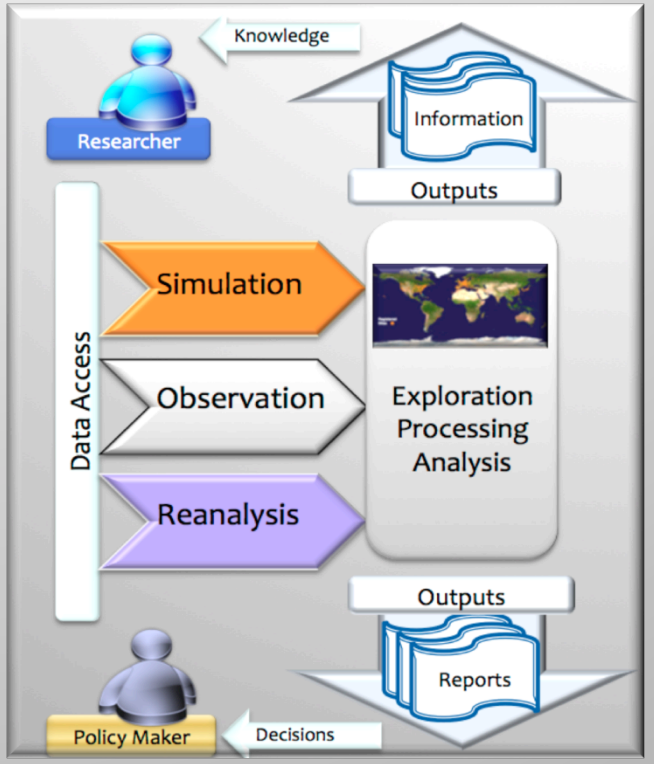
Approach

Free and open consortium of institutions, laboratories and centers around the world that are dedicated to supporting climate change research and its environmental and societal impact.

History

Historically originated from the Earth System Grid (ESG) project, started in 1999, expanded beyond it constituency and mission to include many other projects and partners in the U.S. Europe, Asia, and Australia.

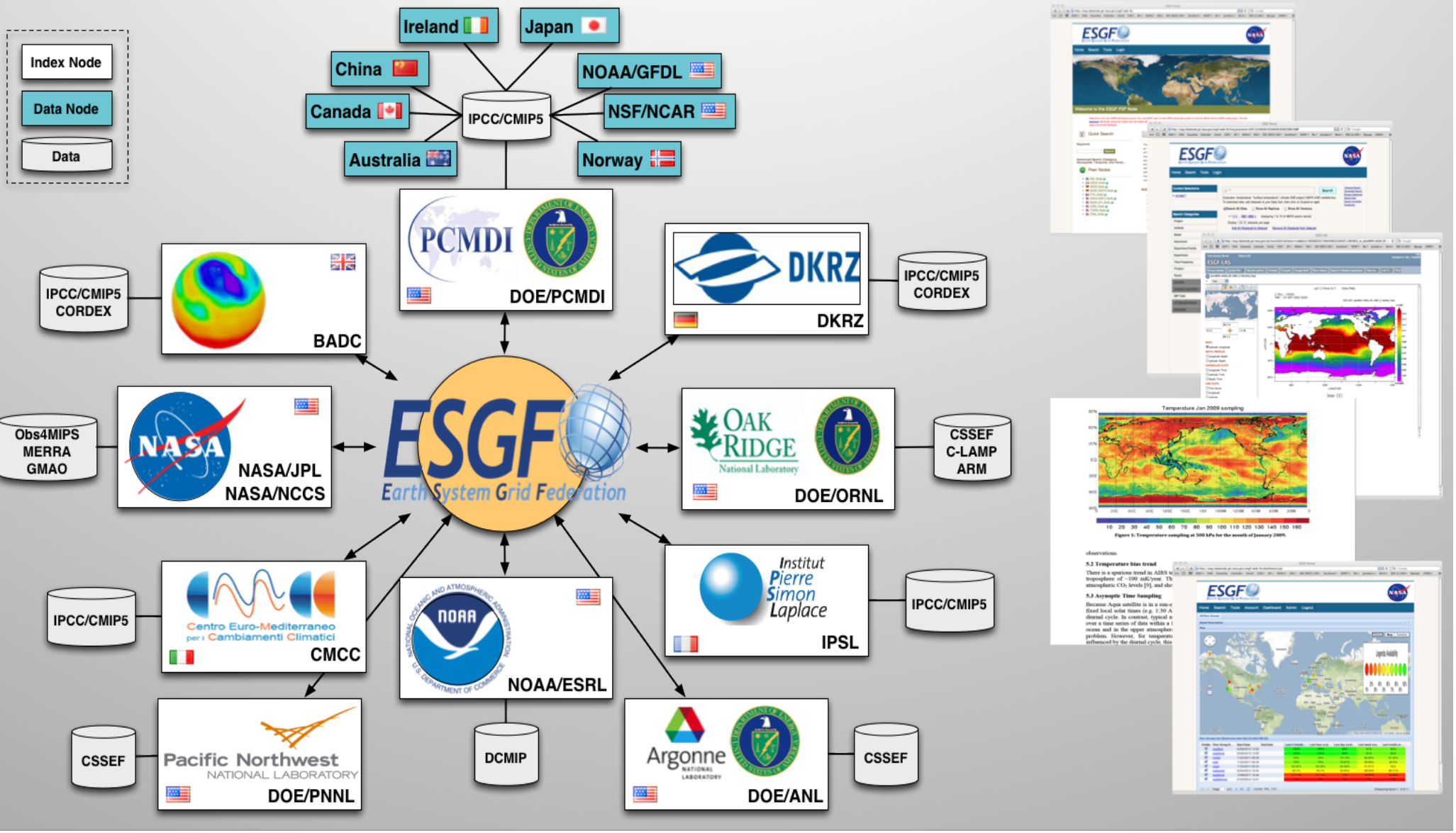




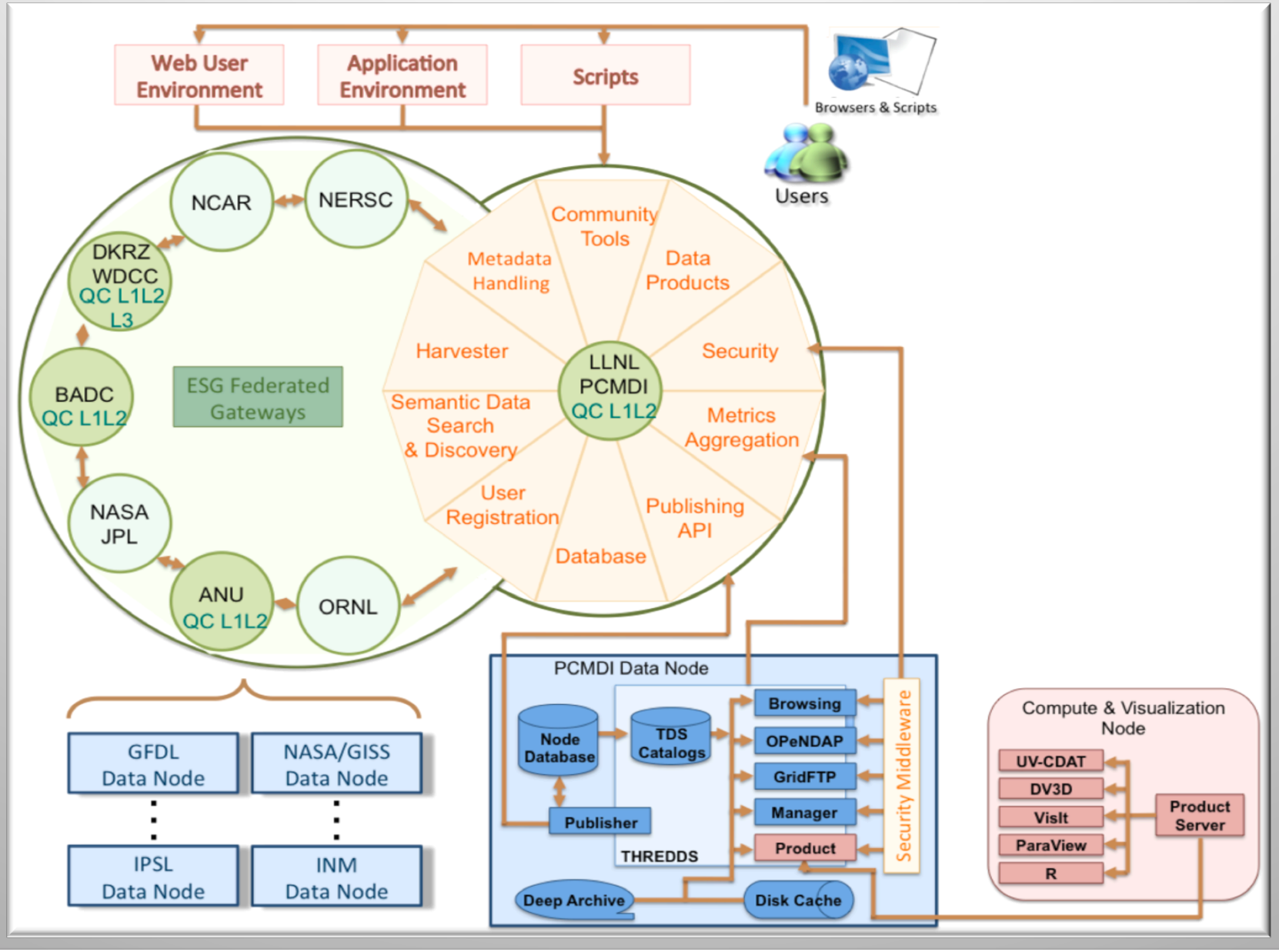
Contributions

Worldwide organizations contributing to the ESGF efforts include: NASA's Observation Intercomparison Project (obs4MIPs); NOAA's Earth System Curator and Global Interoperability Program; EU's MetaFor and Infrastructure for the European Network for Earth System Modeling, and many more.

Federated and Integrated Data from Multiple Sources

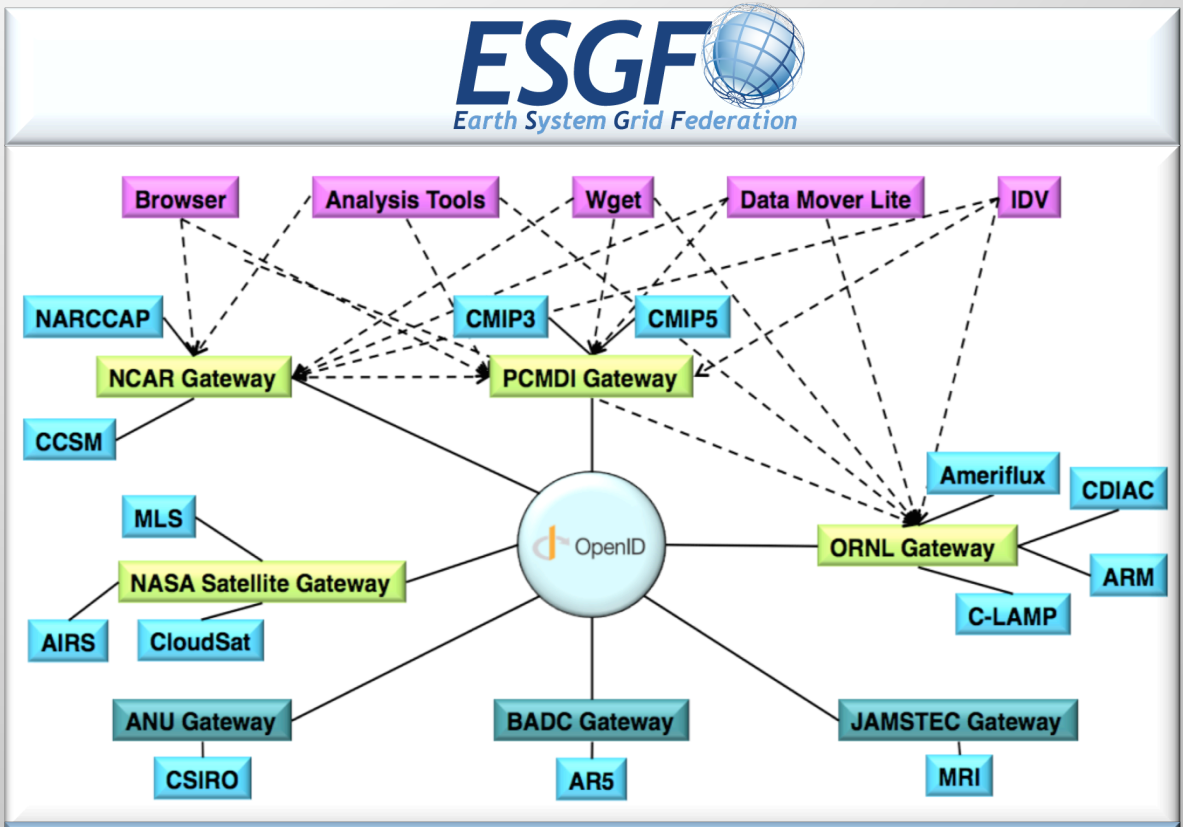


CMIP5 Managed Distributed Archive led by the Earth System Grid Federation (ESGF)



The ESGF Distributed Data Archival and Retrieval System

- Distributed and federated architecture
- Support discipline specific Portals
- Support browser-based and direct client access
- Single Sign-on
- Automated script and GUI-based publication tools
- Full support for data aggregations
  - A collection of files, usually ordered by simulation time, that can be treated as a single file for purposes of data access, computation, and visualization
- User notification service
  - Users can choose to be notified when a data set has been modified



Large amounts of data movement and management are needed for the climate community.

ARM/CDIAC Integration with the Earth System Grid Federation (ESGF)

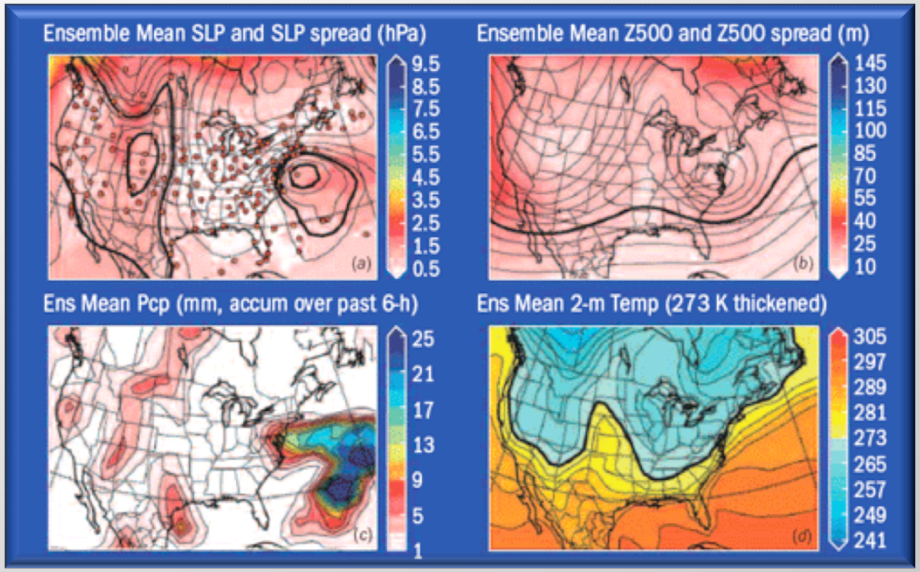
- ARM/CDIAC data set publication plan

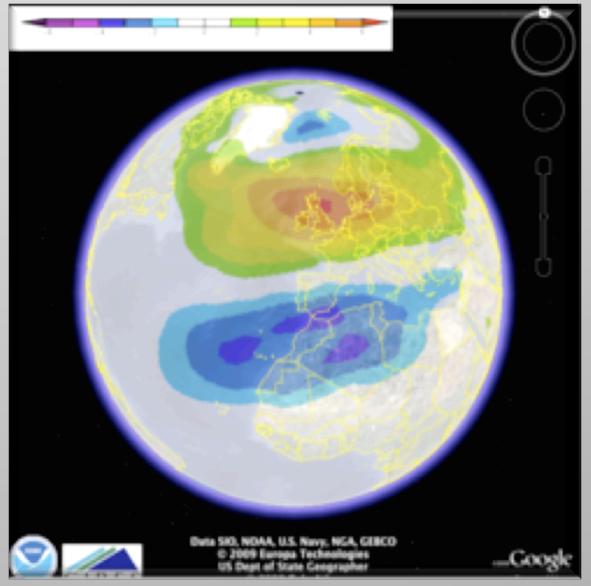
Currently Published	To Be Published
Ameriflux	Balloon-Borne Sounding System
Fossil Fuels	Active Remotely-Sensed Cloud Locations
Obs4MIPs	Microwave Water Radiometer

- Revised workflow for seamless publication of ARM/CDIAC data sets to ESGF
  - ARM/CDIAC centers maintain a THREDDS server containing ESGF-parsable metadata catalogs of native archives
  - An ESGF "Plugin" is built containing:
    - Flexible Publication tools (EZ-Pub)
    - A catalog crawler for ingestion into the ESGF search index to enable data set discovery
    - Modules for data visualization, analysis, and mining
    - Security mechanisms for user authentication and verification
    - Usage metrics and statistics collectors for policy makers and administrators

Reanalysis Integration with the Earth System Grid Federation (ESGF)

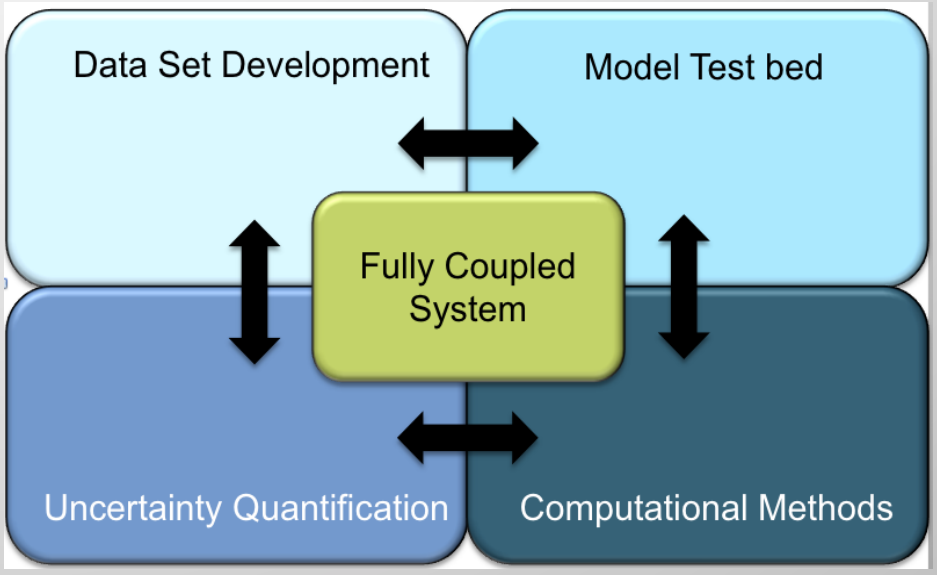
- To enhance climate science resources, NASA Goddard Space Flight Center has agreed to host a subset of the primary reanalysis data on their ESGF node in a similar format to the CMIP5 archive. The ESGF node is managed by the NASA Center for Climate Simulation (NCCS).
- Participating reanalysis institutions:
  - NASA/GSFC/GMAO – MERRA
  - NOAA/NCEP – CFSR
  - ECMWF – Interim
  - JMA/JMA – 25
  - NOAA – 20CR
- Data will need to be translated to the CMIP5 NetCDF/CF format through the CMOR application
- https://oodt.jpl.nasa.gov/wiki/display/CLIMATE/Sharing+Observations+for+Climate+Research



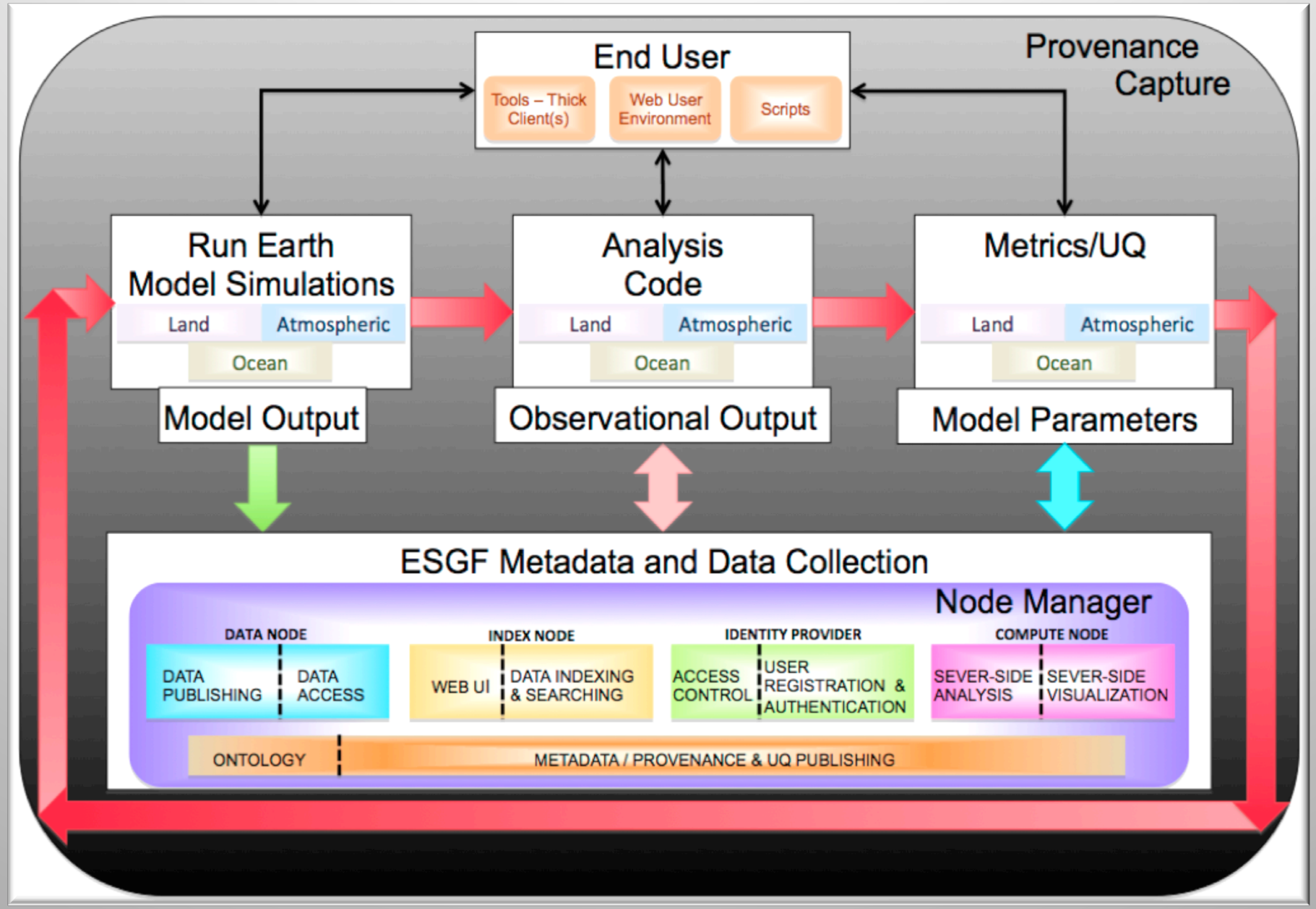


Climate Science for a Sustainable Energy Future (CSSEF)

- **Organization of model component data and scientific needs through the Earth System Grid Federation (ESGF) Peer-to-Peer (P2P) system**
  - Manage existing data and add new data to CSSEF archive
  - Provenance must be documented and retained
  - Stewardship and security
  - Discoverability and accessibility
- **New paradigm**
  - CAM Integration
  - CLM integration
  - Diagnostic calculations on CAM and CLM output integration and publishing results into ESGF
  - Uncertainty Quantification (UQ) calculations on CAM and CLM integration
  - Distribution of workload between clients and "data engines"
  - Automation and capture of workflows for reproducibility and efficiency
  - Documentation of various steps; record script used for publication; note any problems encountered
- **Current projects**
  - Integrate current tools and approaches for test bed and refine for efficiency
  - Test and build from initial subsystem

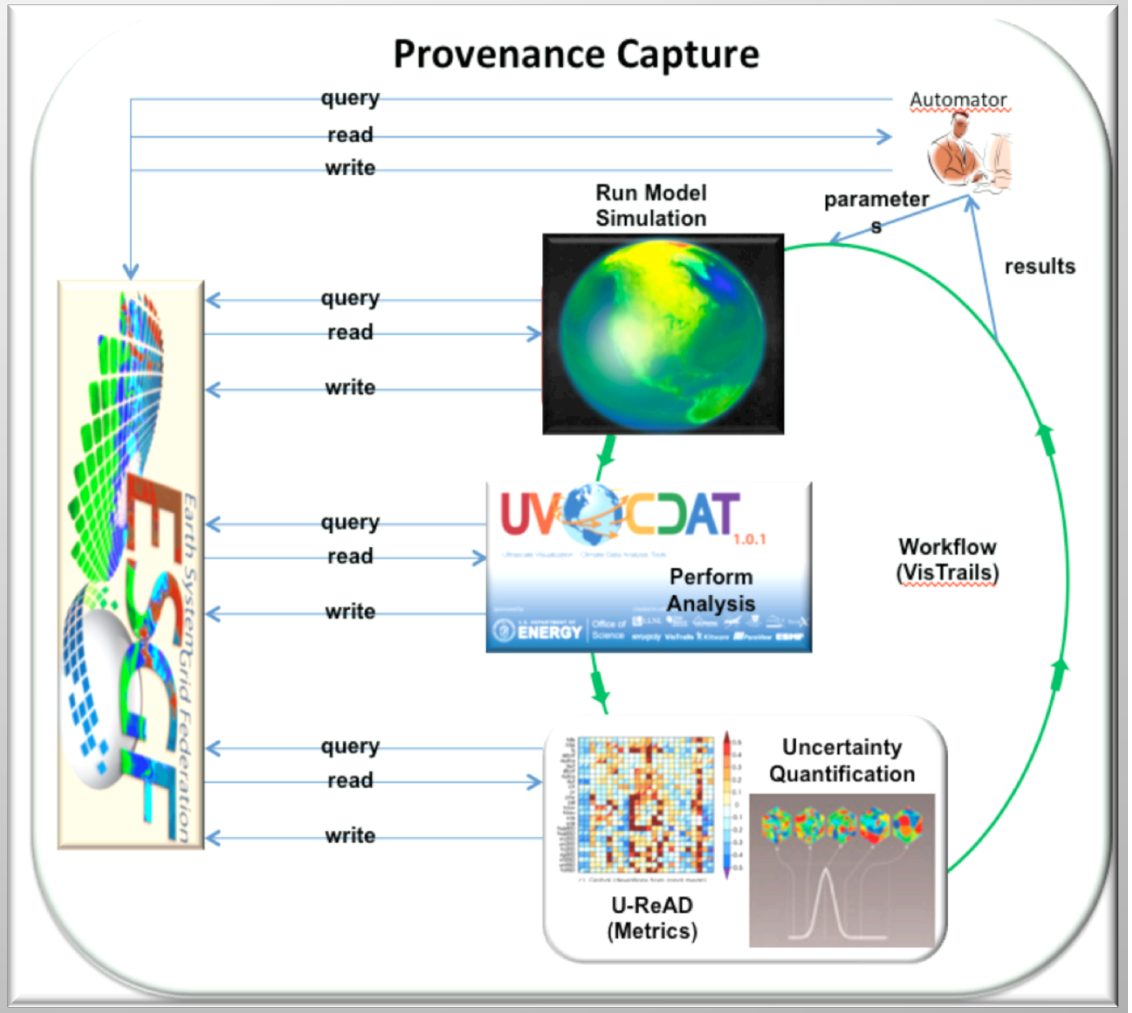


High-level Conceptual View of CSSEF Test Bed Architecture and Workflow



Workflows and Provenance

- **Why Use Workflows in CSSEF?**
  - Standardize scientific experiments, data processing, and analysis under one unified technical approach
  - Workflows will work as building blocks to support more complex problems.
  - Can automatically record what processes executed, what data was used, and what data resulted (Provenance)
- **Why is provenance important?**
  - Without knowing the origin of published data, scientists would have no way to trust the results:
    - What version of the model was used to generate it?
    - What model forcings and parameters were used to produce this result?
    - Real world atmospheric example: LLNL and PNNL both published ARM best estimate data sets. Are they redundant, interdependent or completely independent? The historical record of how they were produced would be the only way to truly differentiate the two efforts.



The Good, the Bad, and the Ugly

- The data centers have generally worked together well
  - with limited resources
  - to design and develop a distributed data archive
  - which has minimized the delay in getting data to users
- The monolithic original software structure has been completely redesigned by the ESG Federation
  - It's called "peer to peer" design (P2P)
  - Increased modularization will speed improvements
  - Increase flexibility will better meet the needs of a diverse user base
- The new web-based user interface substantially
  - Improves speed, accuracy, and flexibility of searches
  - Minimizes clicks
- It is now possible to script downloads without first accessing the web interface

"ESGF P2P release version" is used in production now and running along side the old system until the end of July."

- Increase speed of downloads
  - More nodes will establish gridftp servers (~10x faster than http)
  - Data will replicated at major data centers with generally better performance
- Reduce error rates for downloads and simplify scripting
- Make available all model and experiment documentation
  - Table of forcings for each model & experiment
  - Table of parent experiments and branch times for each realization
  - All information recorded through the METAFOR questionnaire

Near Future

This should happen before the end of summer

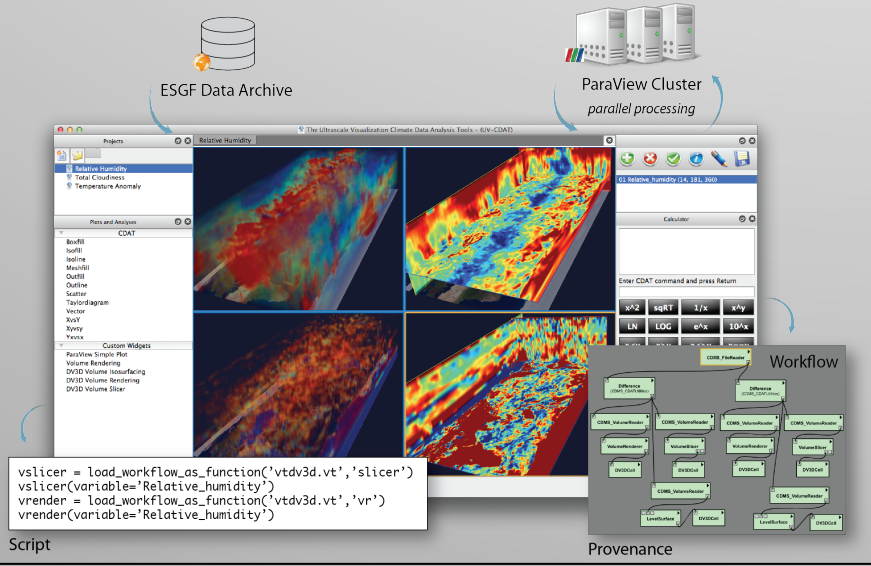
- Data error reports/notification (rudimentary pages now in place) http://cmip-pcmdi.llnl.gov/cmip5/errata/cmip5errata.html
- Service to notify users when new data sets of interest become available.
- Place to record and access CMIP5 publications (web-based form ready now)
- Citable record of CMIP5 provenance (doi assignment and other options)
- Sub-setting of files before download (and other server-side calculations) – better integration with the UV-CDAT is currently underway
- Obs4MIPs: An effort to make observational data that can be directly compared with CMIP5 model output
  - Promoted by Duane Waliser, Robert Ferraro, and others at JPL with cooperation from PCMDI and encouragement from the WGCM
  - Data written in same structure and format as CMIP5 model output
  - Data obtainable through ESGF (product=Obs4MIPs)
  - First products from NASA and from ARM now available
  - ESA and NOAA have expressed interest in contributing
  - Wiki describing Obs4MIPs now visible at: http://obs4mips.llnl.gov:8080/wiki
- ANA4MIPs: A parallel effort is underway to make reanalysis products available (currently NASA MERRA)
  - Promoted by Jerry Potter, and others at Goddard with cooperation from PCMDI and encouragement from the WGCM
  - Data written in same structure and format as CMIP5 model output
  - Data obtainable through ESGF (product=ANA4MIPs)

BER Supported Data Activities

http://uvcdat.llnl.gov

Ultra-scale Visualization Climate Data Analysis Tools (UV-CDAT)

- Integrate DOE's climate modeling and measurements archives
- Develop infrastructure for national and international model/data comparisons
- Deploy a wide-range of climate data visualization, diagnostic, and analysis tools with familiar interfaces for very large, high resolution climate data sets (CDAT, VTK, R, VisIt, ParaView, DV3D, …)
- Workflow – data flows are directed graphs describing computational tasks
- Takes advantage of ESGF data management



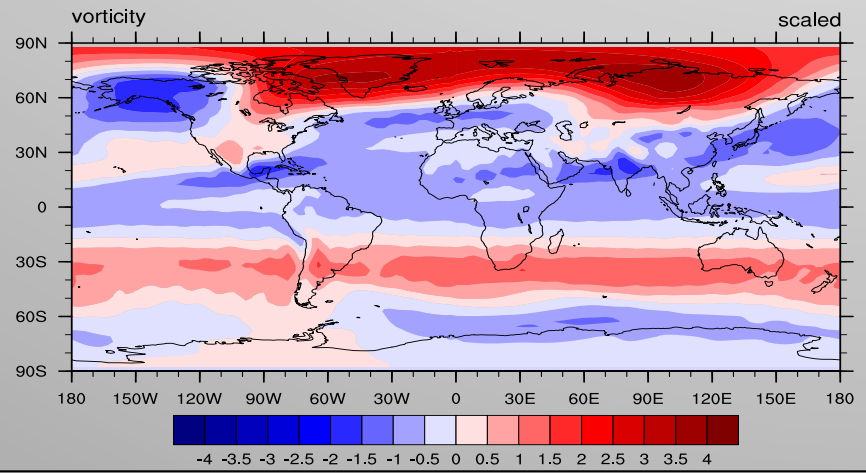
Visual Data Exploration & Analysis of Ultra-large Climate Data

- Climate applications, in which specific case studies aimed at answering climate change questions will provide the science drivers for technology development;
- Technology adaptation, where applied research is performed to extend existing technologies to meet the needs of the science drivers; and
- Software engineering and integration is carried out to deliver working tools to the climate community.

BER Supported Data Activities

Parallel Analysis Tools and New Visualization Techniques for Ultra-Large Climate Data Sets

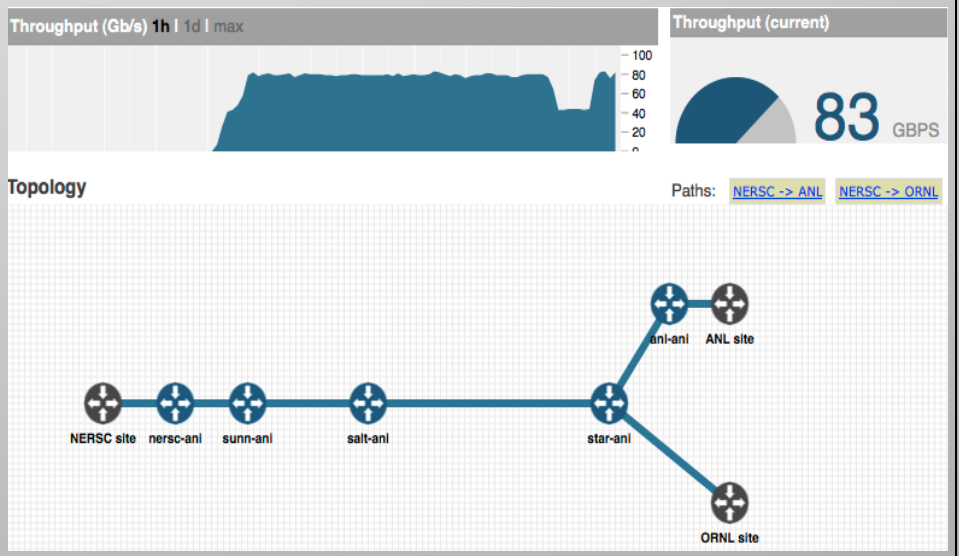
- Speed up current diagnostics (e.g the CESM-CAM atmospheric model diagnostics) with task parallelism
- Create a data-parallel version of the NCAR Command Language (NCL) analysis and visualization package.
- Build a new library: ParCAL – Parallel Climate Analysis Library.
- Use existing software technology (MOAB, PnetCDF, Intrepid).
- ParNCL (built with ParCAL) will allow users to run their NCL scripts unaltered.
- Explore news ways of doing 3D visualization of climate data



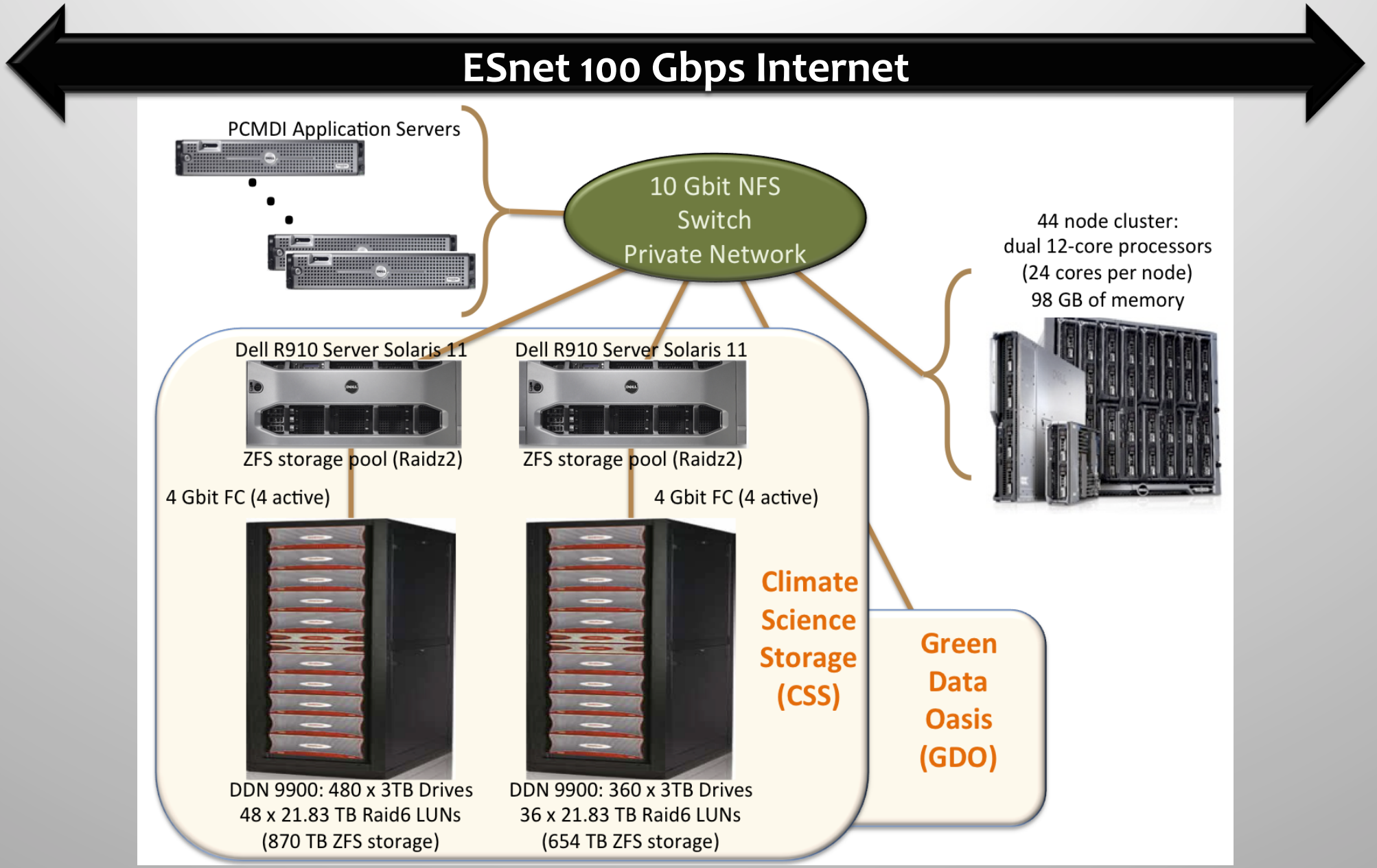
Climate100: Scaling Climate Applications to 100 Gbps Network

- Total size of data is increasing.
- There are many files, relatively small files, in climate data sets.
- It requires efficient methods to fully utilize the underlying network infrastructure with limited resources.
- Averaging 83Gbps on average over TCP connections.
- The 100Gbps network is in the testing phase. (Expected to be in production by the end of 2012.)

https://sdm.lbl.gov/climate100



BER Funded Climate-science Storage System with Scalable Compute Clusters



BER "Climate K-Base": Bring Together Large Volumes of Diverse Data to Generate New Insights

Data integrating enterprise system

Insight into big data reveals three very significant challenges:

- **Variety:** managing complex data, including storage and retrieval, from multiple regional and non-regional data indices, types and schemas
- **Velocity:** distributing live data streams and large volume data movement quickly and efficiently
- **Volume:** analyzing large-volume data (from terabytes to zettabytes) in-place for big data analytics

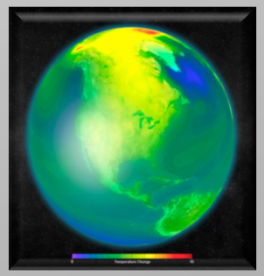
BER invests in:

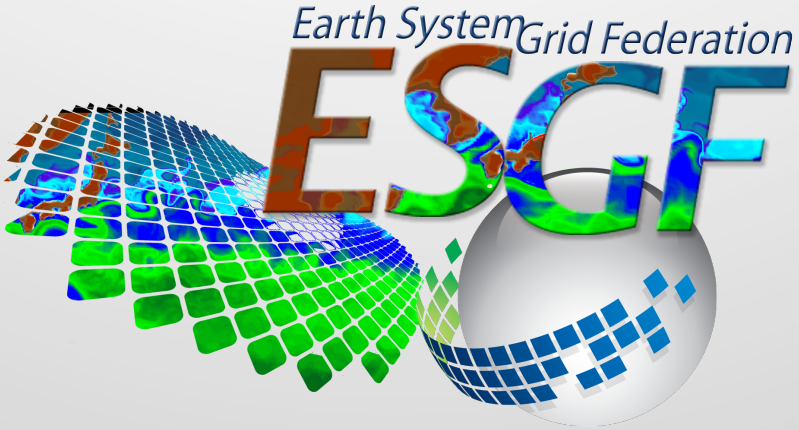
- **Accessing Global Information:** Accessing climate data and content information from everywhere via the web, sensors, and applications in an integrated and federated environment
- **Flexible Infrastructure:** Flexible automated administration, easy-to-use analytics, and virtualization at every level
- **Scalable Framework:** Big data analytics in a scalable environment with efficient parallelism, workload-optimization, and real-time streaming process

Simulation

Observation

Reanalysis

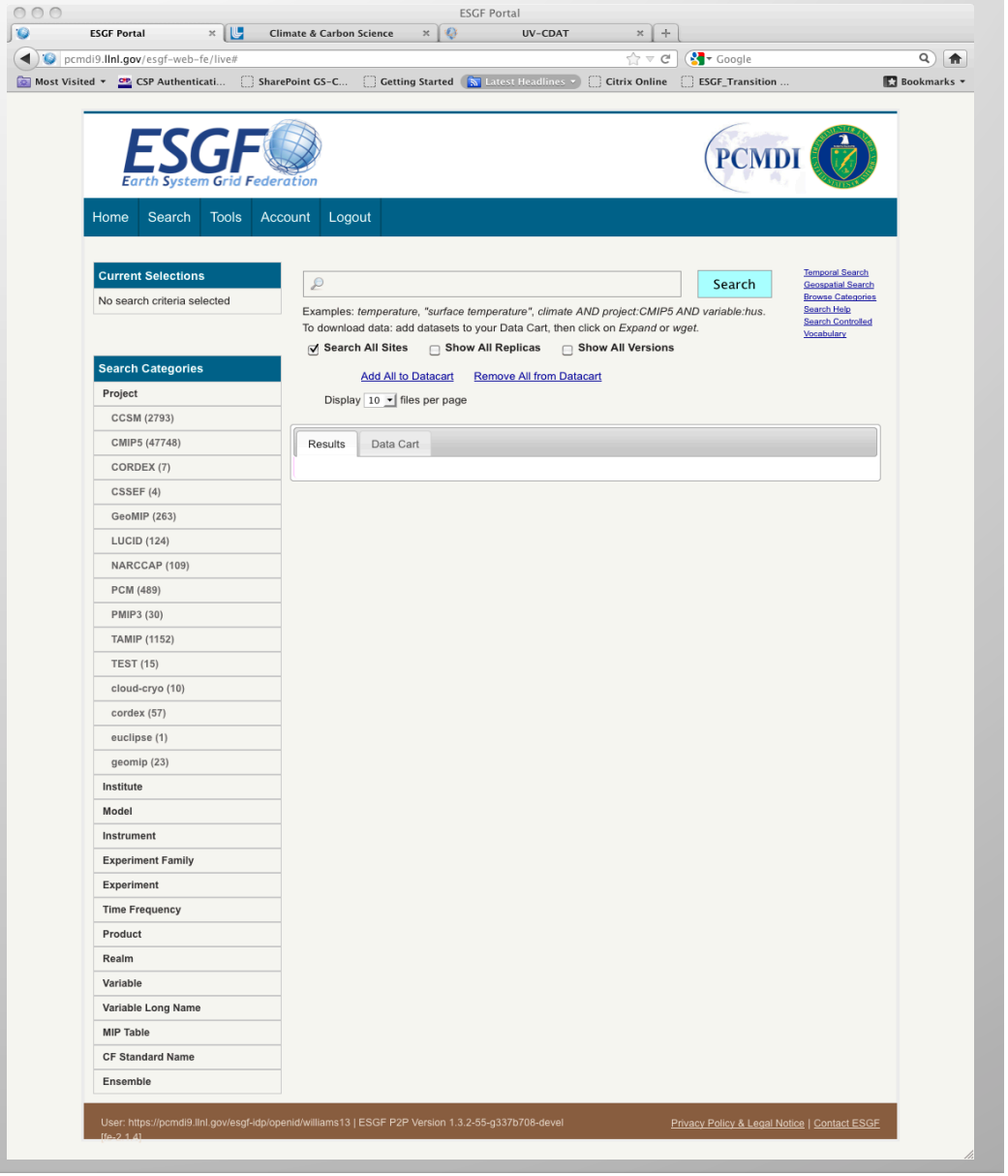




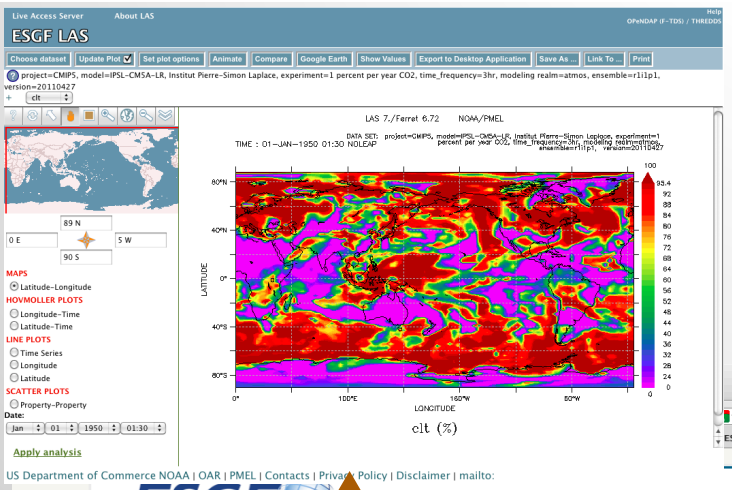
BACKUP SLIDES

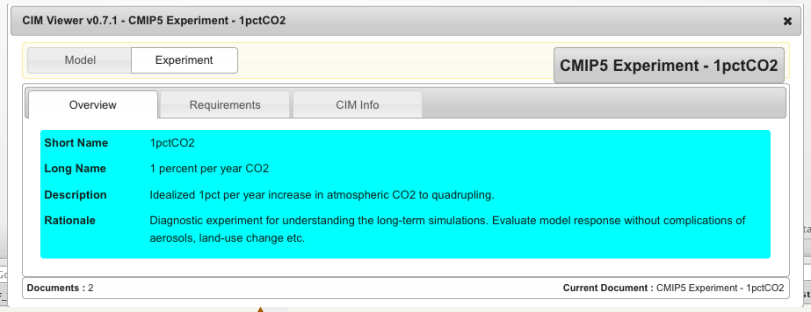
ESGF Web Front-End

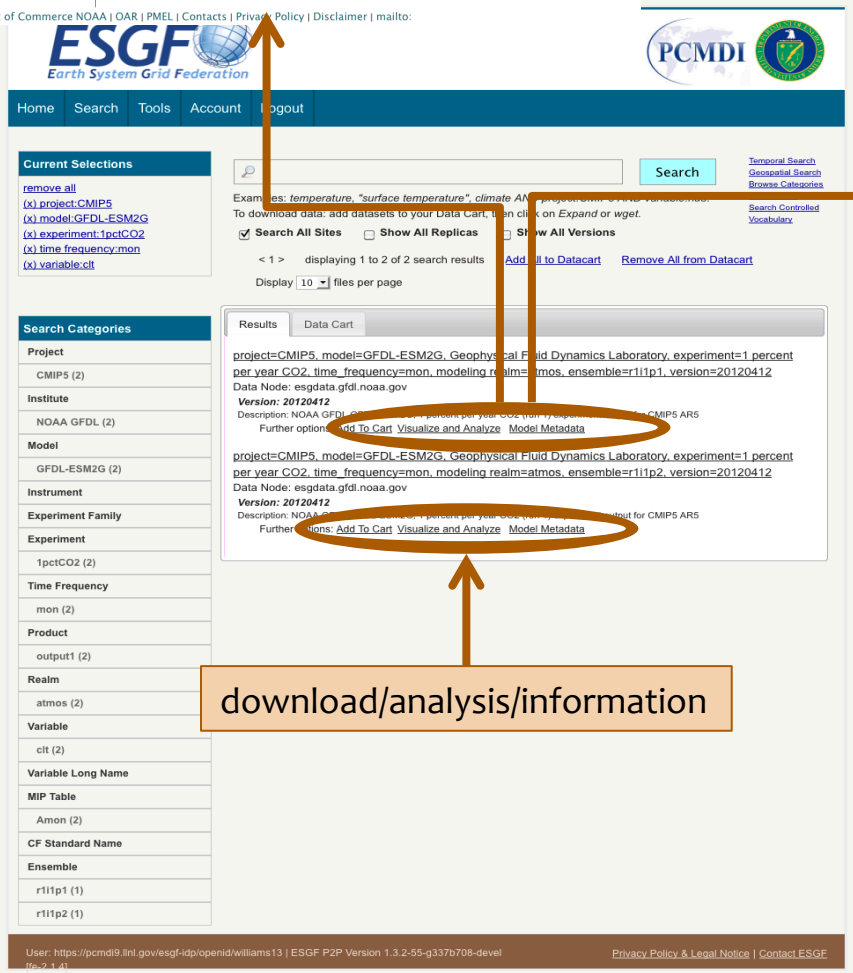
http://pcmdi9.llnl.gov



ESGF Web Front-End





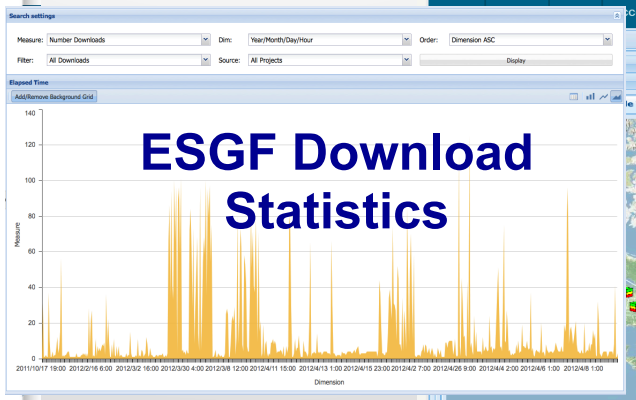


download/analysis/information

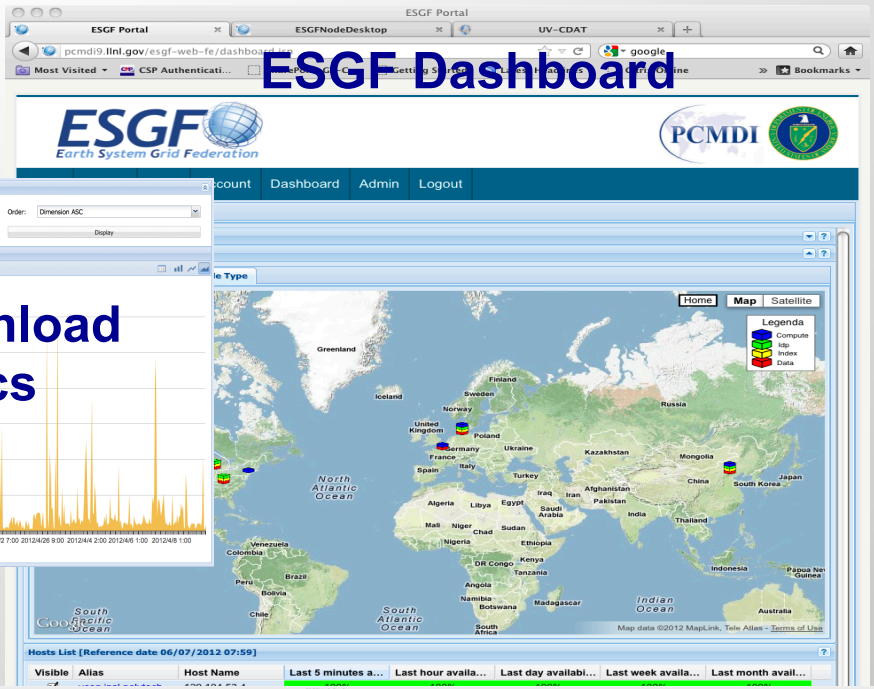
Download apps

ESGF Web Front-End

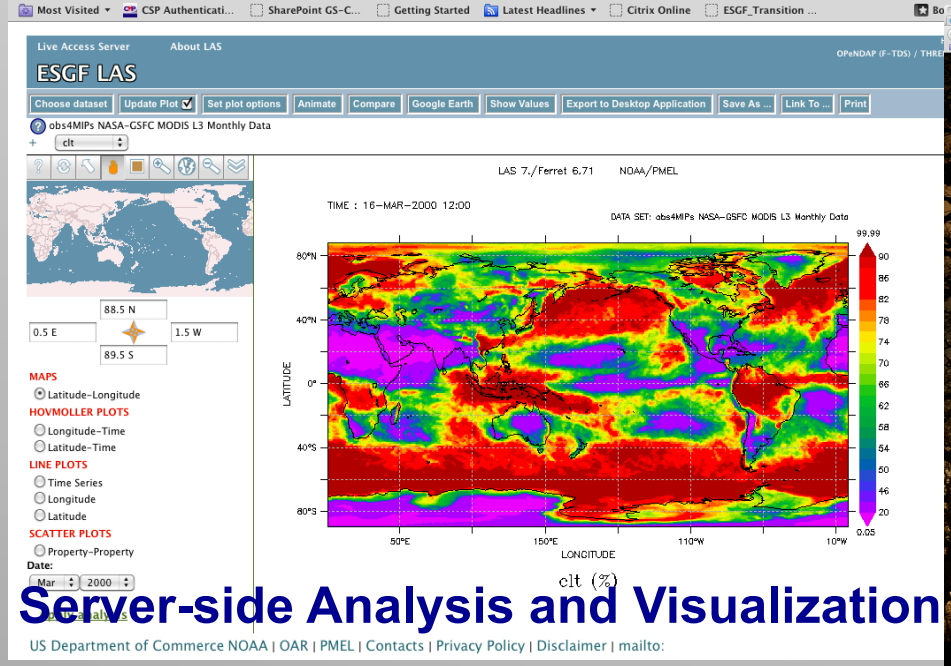
Geospatial Search



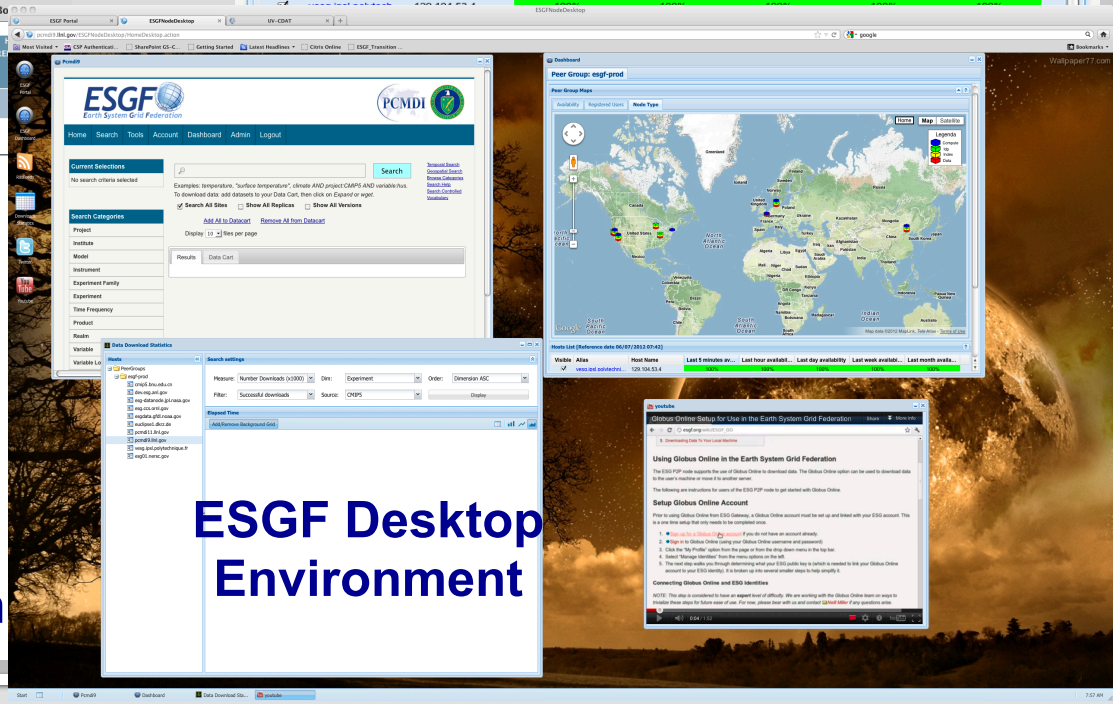
ESGF Download Statistics



ESGF Dashboard



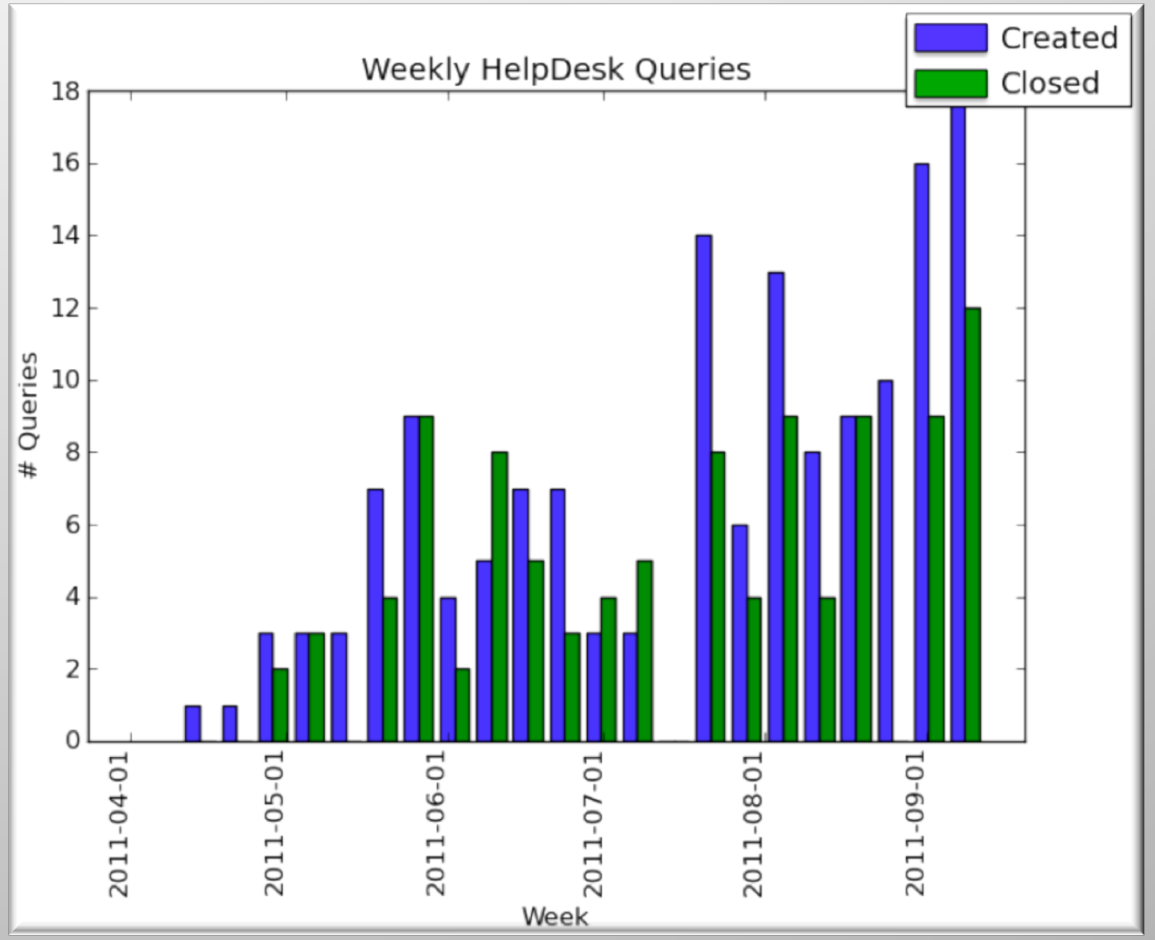
Server-side Analysis and Visualization



ESGF Desktop Environment

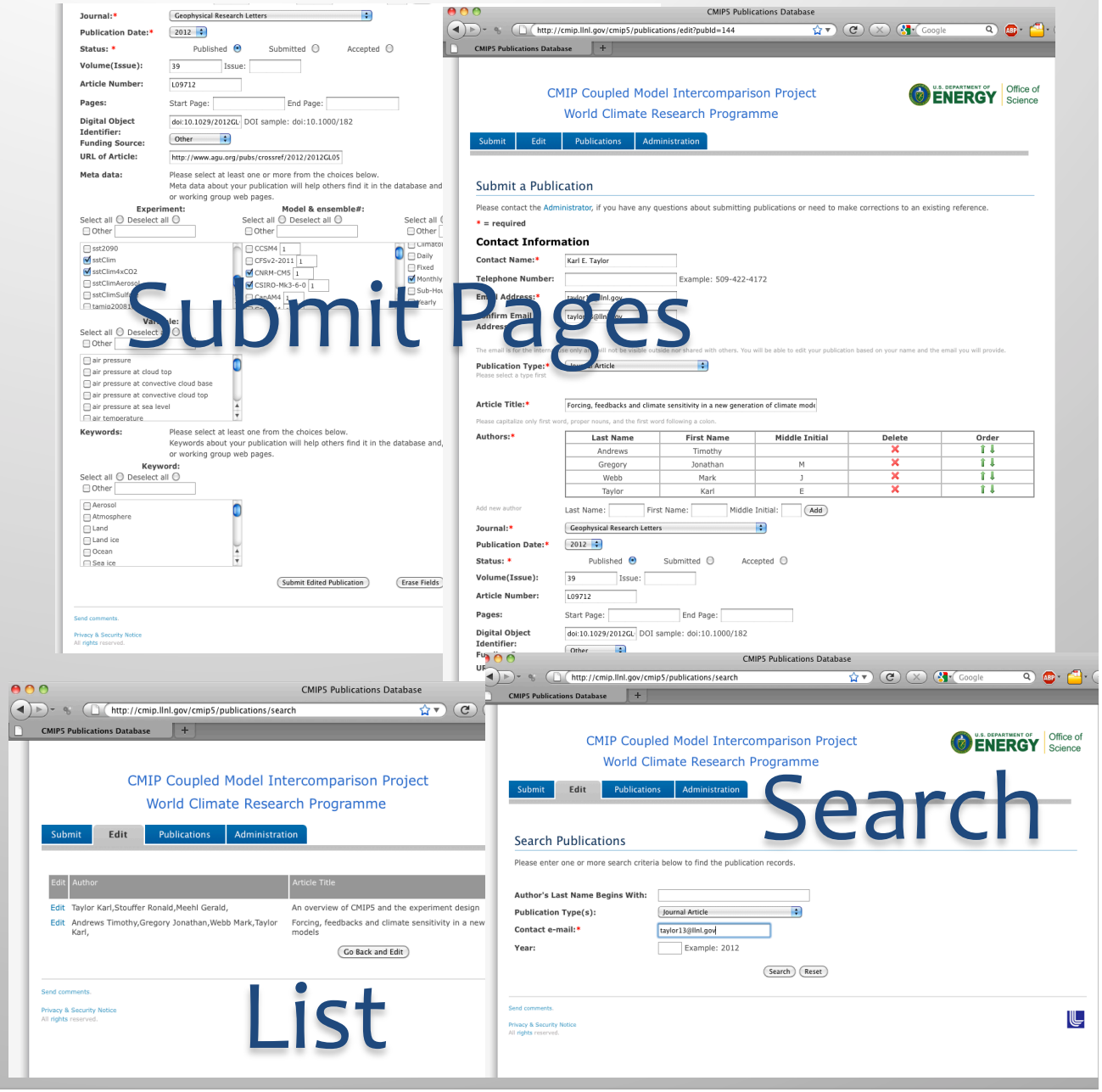
ESGF Help Desk Weekly Traffic

- About half of these queries come directly to **cmip5-helpdesk@stfc.ac.uk** and the other half to the esg-support mailing list **esgf-user@lists.llnl.gov**
- Questions that are resolved are place on the **ESGF FAQ** list
- **Scientists** at PCMDI/LLNL, BADC, and DKRZ are charged with addressing CMIP5 data questions
- **Technical staff** at LLNL, BADC, DKRZ, NCAR, and JPL are charged with addressing ESGF system questions

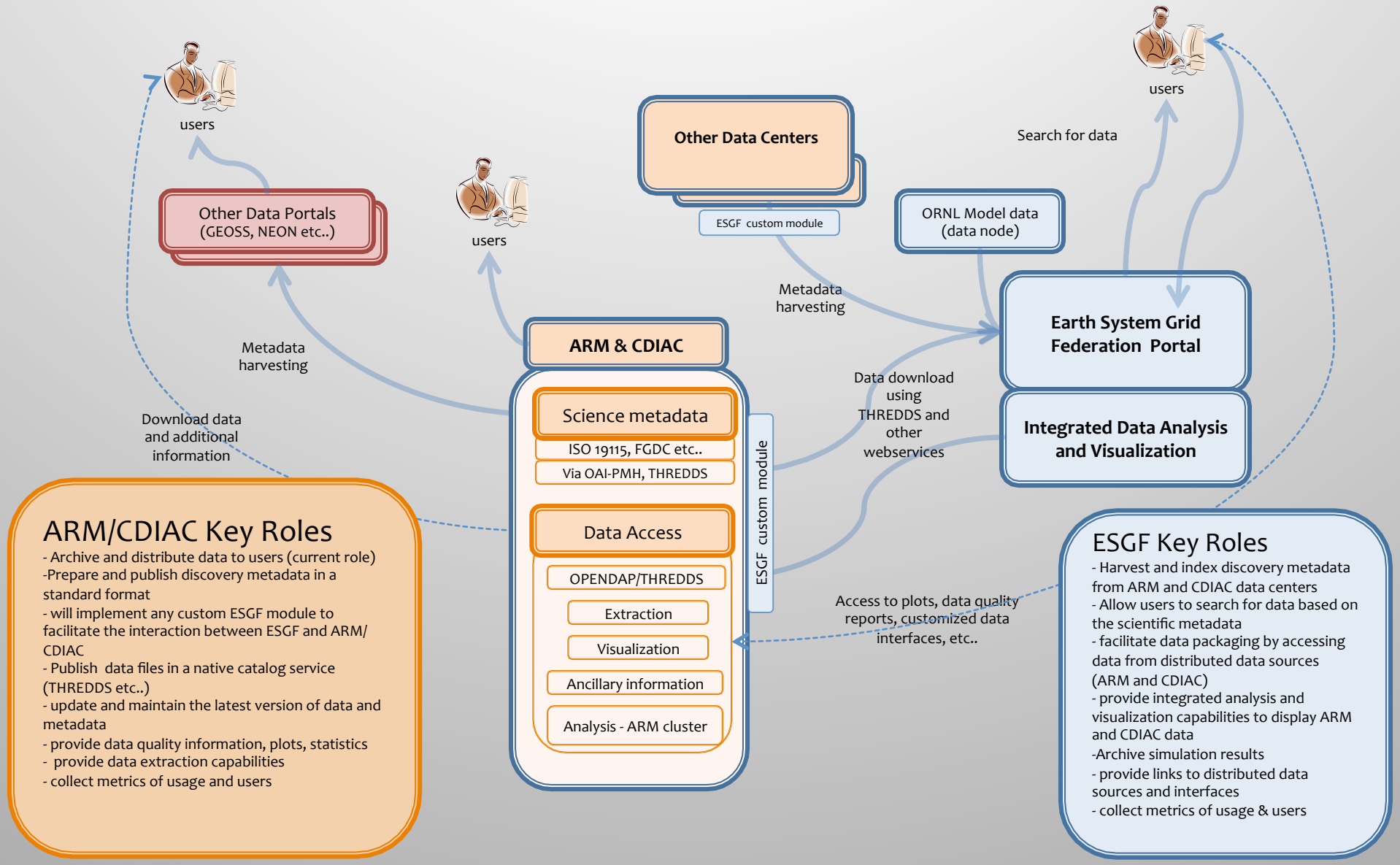


Publication Web Application

- **Web based submission** of citations to database
- **Capture tags** to enable contextual search, the tags include
  - Keywords
  - Funding
  - Data used (model, experiment, variable, time frequency)
- Submission page differentiate with the **journal type**
  - The types are: journal, book, proceeding, presentation, technical report
- **Editable database** entry
  - Enable search of all submitted publications, update, change or add keywords
- Admin page for **editing** or removing publications

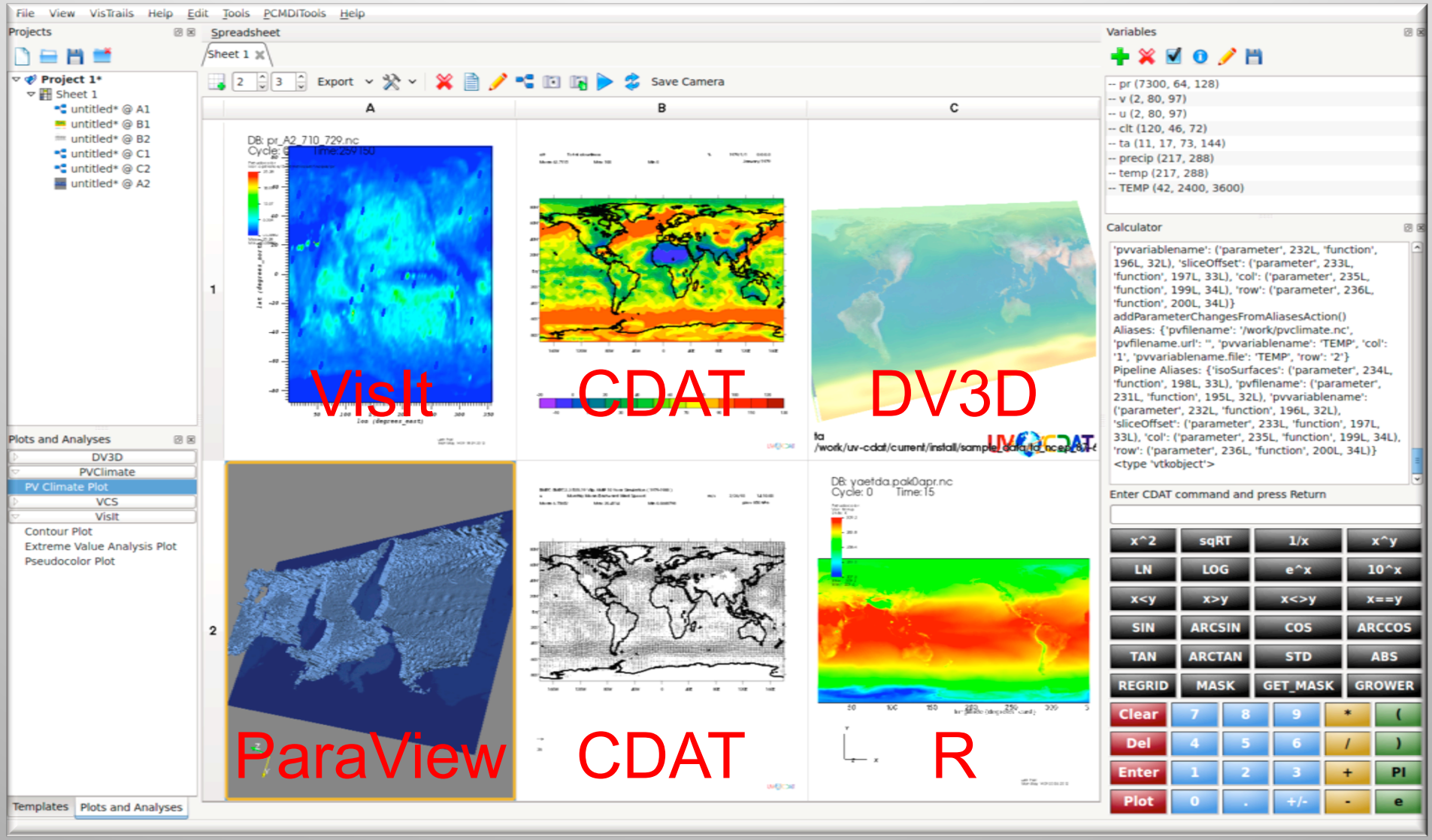


ESGF – ARM and CDIAC Publication Architecture



Ultra-large Climate Data Analysis and Visualization
UV-CDAT Displaying CDAT, DV3D, ParaView, VisIt, and R

http://uvcdat.llnl.gov



Layered Data Distributed Open Architecture