LLNL-PRES-575652

Prepared by LLNL under Contract DE-AC52-07NA27344.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Security, LLC, Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

U.S. DEPARTMENT OF ENERGY | Office of Science

Climate Science Responds to "Big Data" Challenges: Accessing Analyzing Model Output and Observations

February 15, 2013

Dean N. Williams

On behalf of Multiple Earth System Communities and Projects

ESGF Earth System Grid Federation

UV-CDAT

SAMSI/NCAR Workshop on Massive Datasets in Environment and Climate

Overview: Bring together large volumes of diverse data

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 exabytes) in-place for **big data analytics**

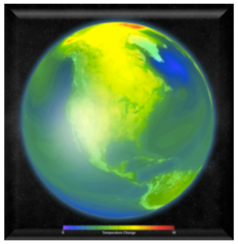
Community invests in:

- **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

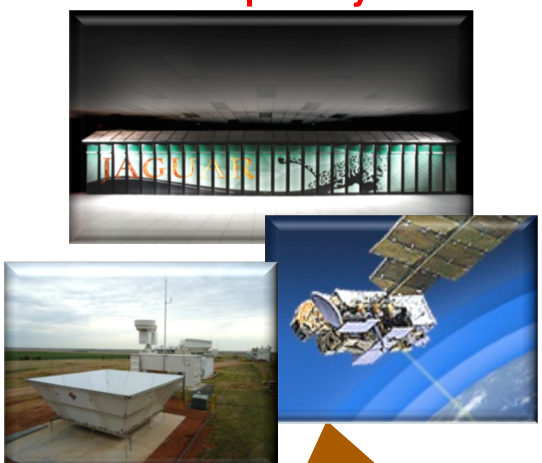


Predictive analysis of complex systems

Collection and data management
- Sensors
- Data models
- Transport/comm
- Storage and provenance

Pattern discovery
- Descriptive statistics
- Graph analytics
- Machine learning
- Signal and image processing

Critical complex systems



Data-intensive computing
- Architectures – persistent data to streams
- Programming environments
- Human-computer interface

Predictive models
- Statistical prediction-classification-anomaly detection
- Steering discrete-event/ continuous simulations

Decisions and control
Design optimization
Policy making
(Humans)

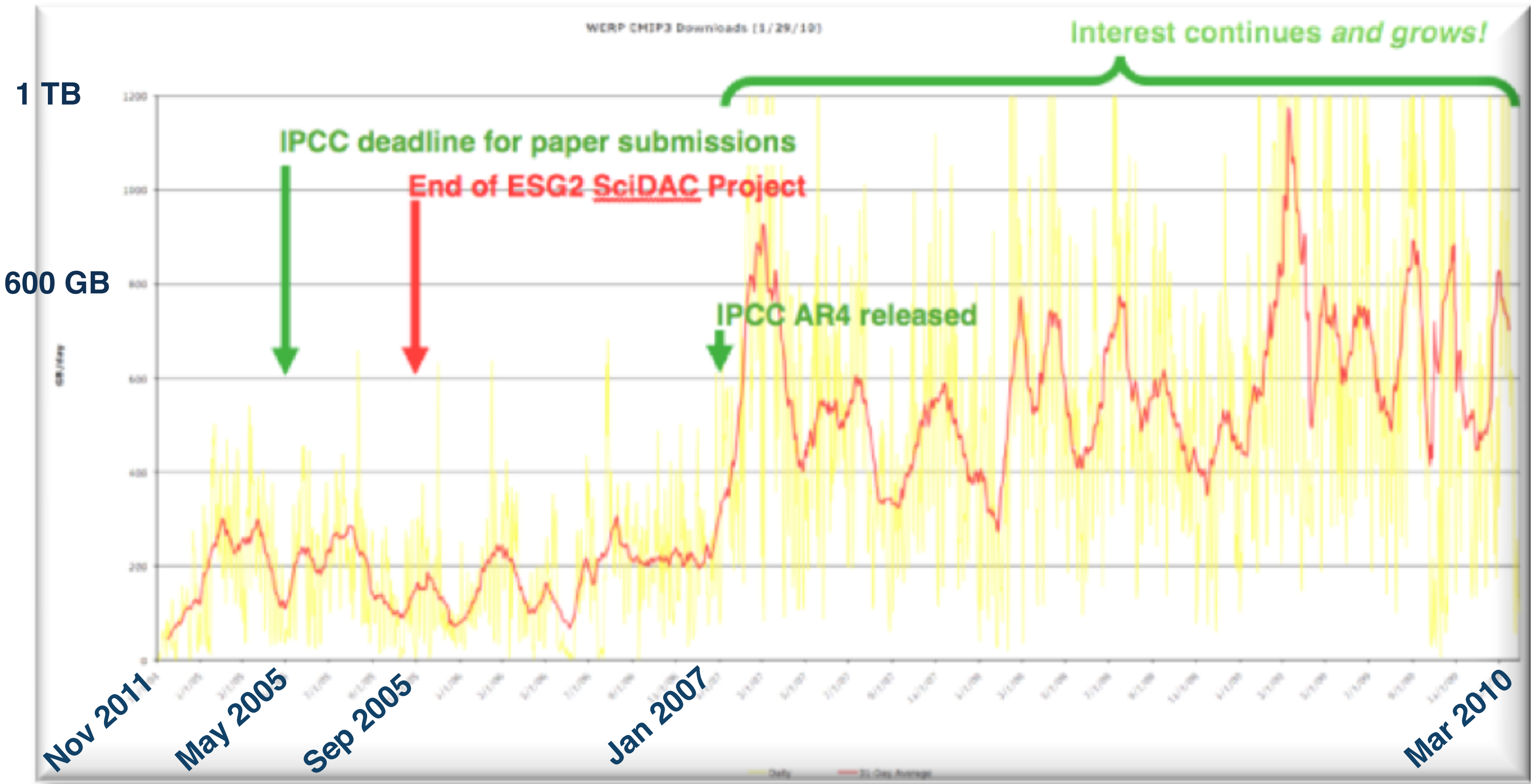
Example Project: The CMIP experiment design

CMIP5: 62 models available from 25 centers

- CMIP = Coupled Model Intercomparison Project
  - Phase 1: Idealized simulations of present-day climate (~1 Gigabyte (GB))
  - Phase 2: Idealized simulations of future climate changes (~500 GB: CMIP2/CMIP1=500)
  - Phase 3: More realistic simulations (2004 – present) (~35 Terabytes (TB): CMIP3/CMIP2 = 70)
- CMIP 5 multi-model archive expected to include (3.5 Petabytes (PB) CMIP5/CMIP3 = 100):
  - 3 suites of experiments
  - 25modeling centers in 19 countries
  - 60+ models
  - Total data, ~3.5 PB
  - Replica 1 – 2 PB
  - Derived data ~1 PB
- Global distribution
- Timeline fixed by IPCC (2012 - 2013)
- The community organizes, manages and distributes the CMIP/IPCC (Intergovernmental Panel on Climate Change) database of climate model output
- CMIP6 (350 PB – 3 EB ?)

kilobyte (kB)	10^3
megabyte (MB)	10^6
gigabyte (GB)	10^9
terabyte (TB)	10^{12}
petabyte (PB)	10^{15}
exabyte (EB)	10^{18}
zettabyte (ZB)	10^{21}
yottabyte (YB)	10^{24}

CMIP3 (IPCC AR4) download rates in gigabytes per day



Data challenge of CMIP3 archive vs. CMIP5 archive

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

Archive size: 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
CESM	USA	739
NCC	Norway	32
NCEP	USA	26
NIMR/KMA	Korea	14
NOAA GFDL	USA	158
Totals		3,108 (PB)

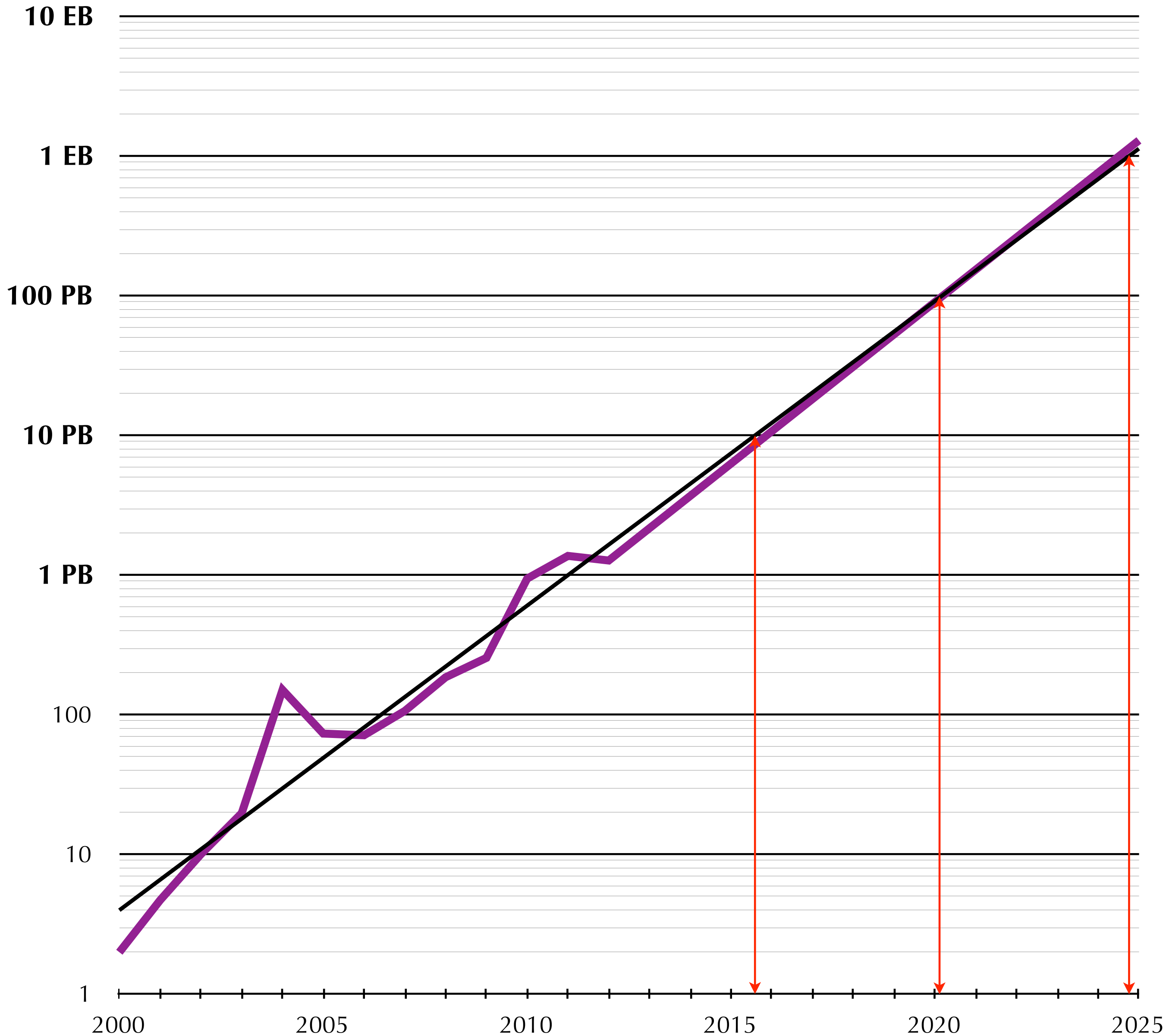
Archive size:
currently: 1.4 PB
total: 3.1 PB by 2013

CMIP5/CMIP3 = 10^2

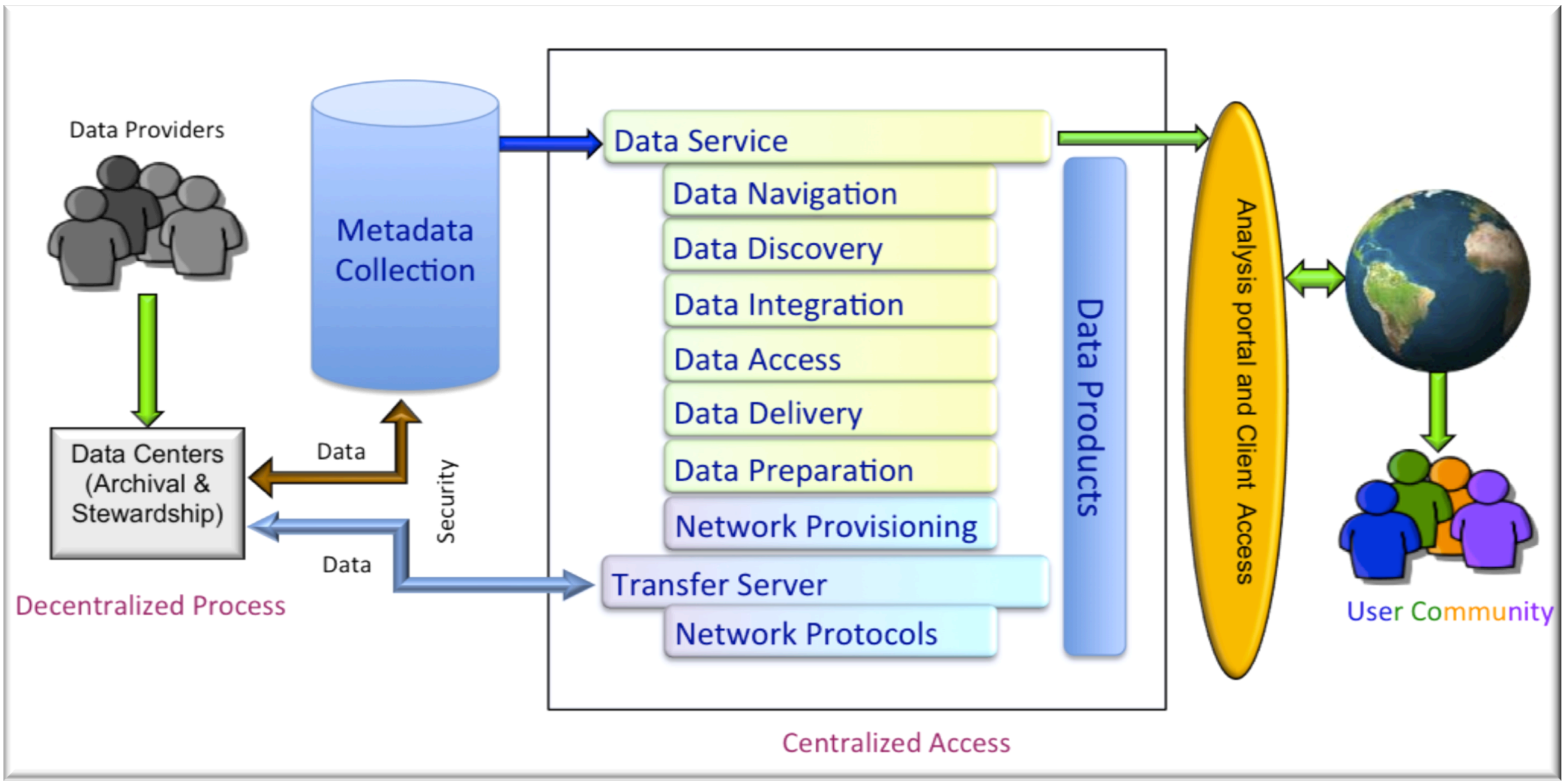
Focus on the U.S. climate model simulation output.

Projected DOE/NSF CESM output

year	total (TB)
2000	2
2001	5
2002	10
2003	20
2004	150
2005	73
2006	71
2007	106
2008	185
2009	254
2010	940
2011	1,366
2012	1,266
2013	2,158
2014	3,676
2015	6,264
2016	10,672
2017	18,184
2018	30,983
2019	52,792
2020	89,950
2021	153,263
2022	261,139
2023	444,946
2024	758,128
2025	1,291,749
2026	2,200,967
2027	3,750,154
2028	6,389,762
2029	10,887,300
2030	18,550,504

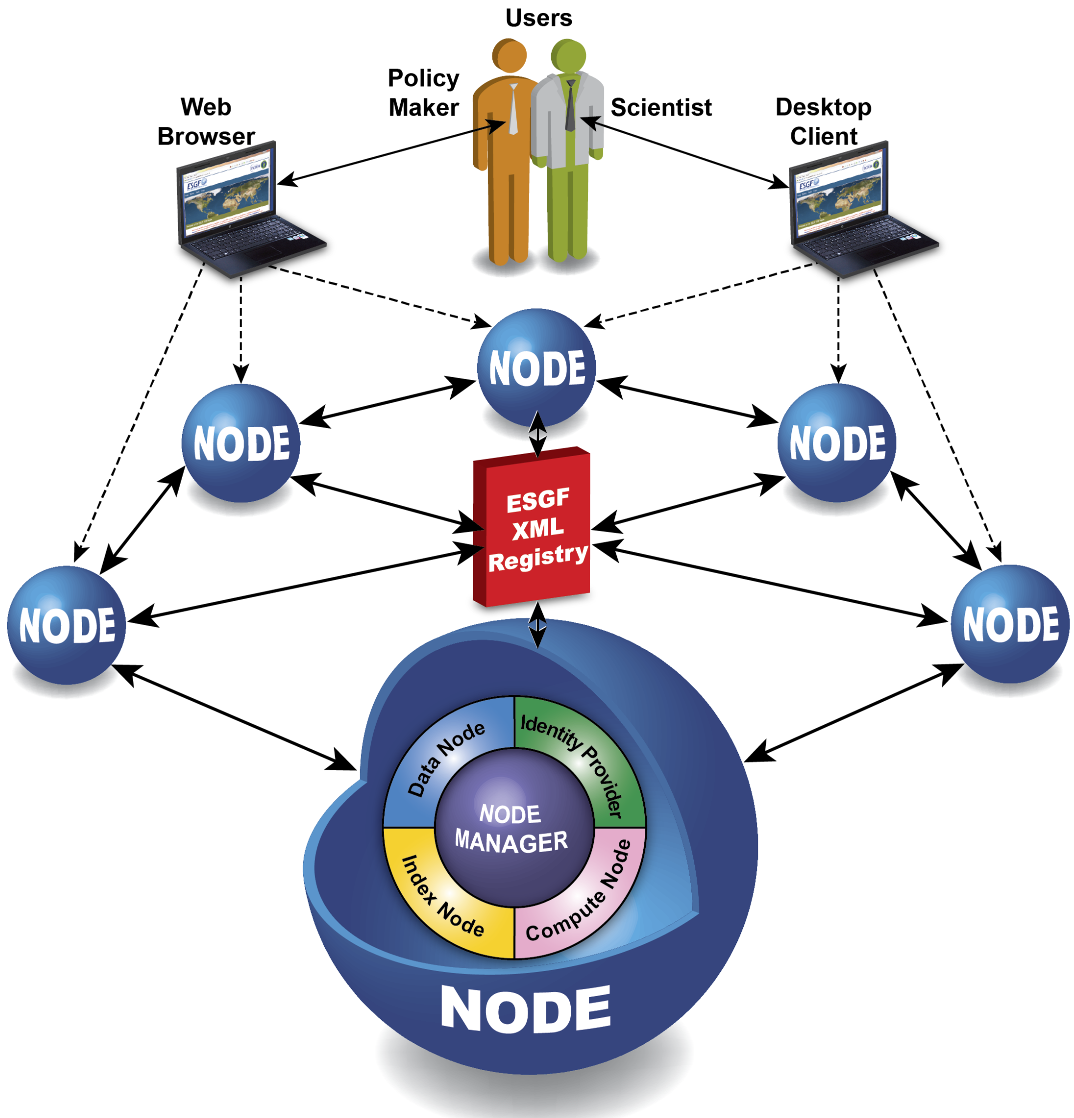


Cloud type approach for distributed data

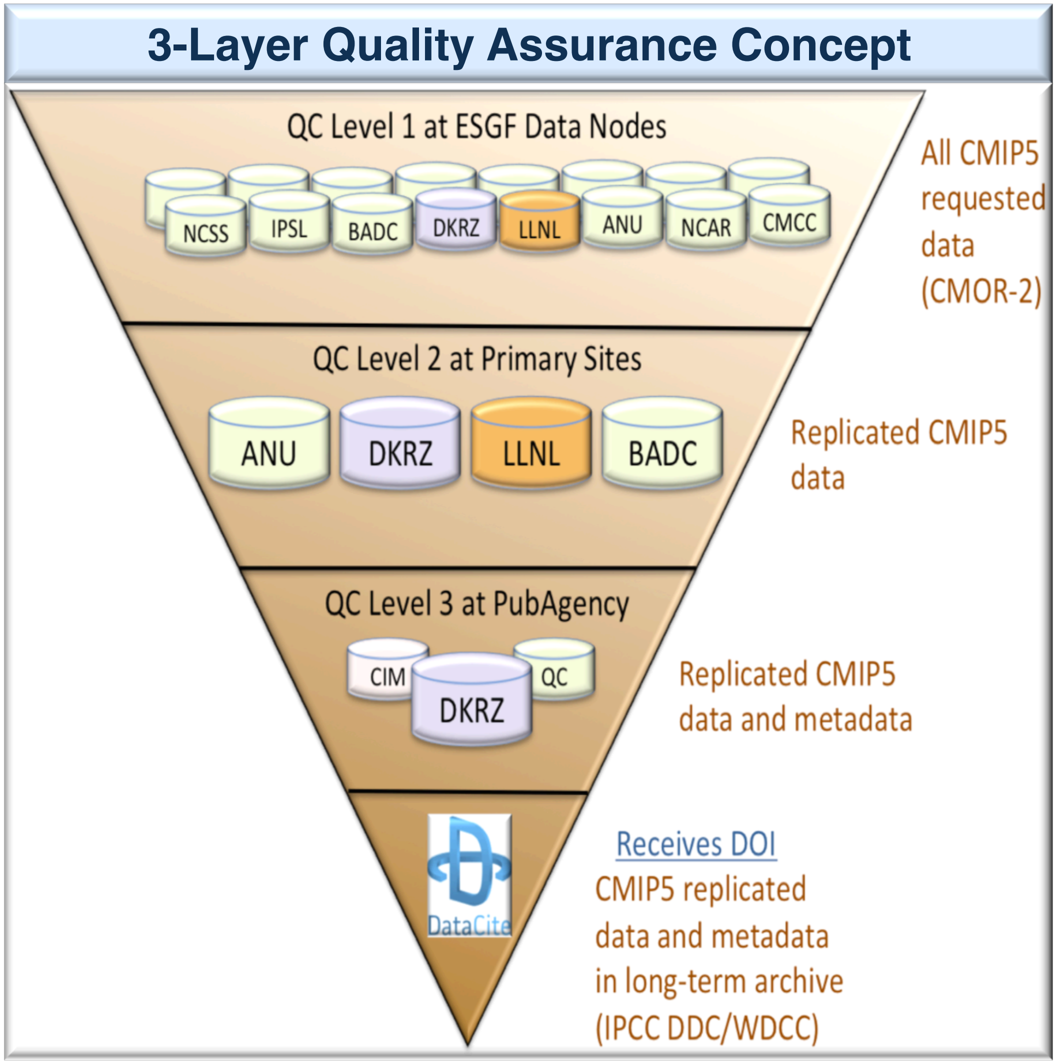


The Earth System Grid Federation (ESGF) distributed data archival and retrieval system

- 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



Data quality control check operations end in digital object identifiers (DOIs)



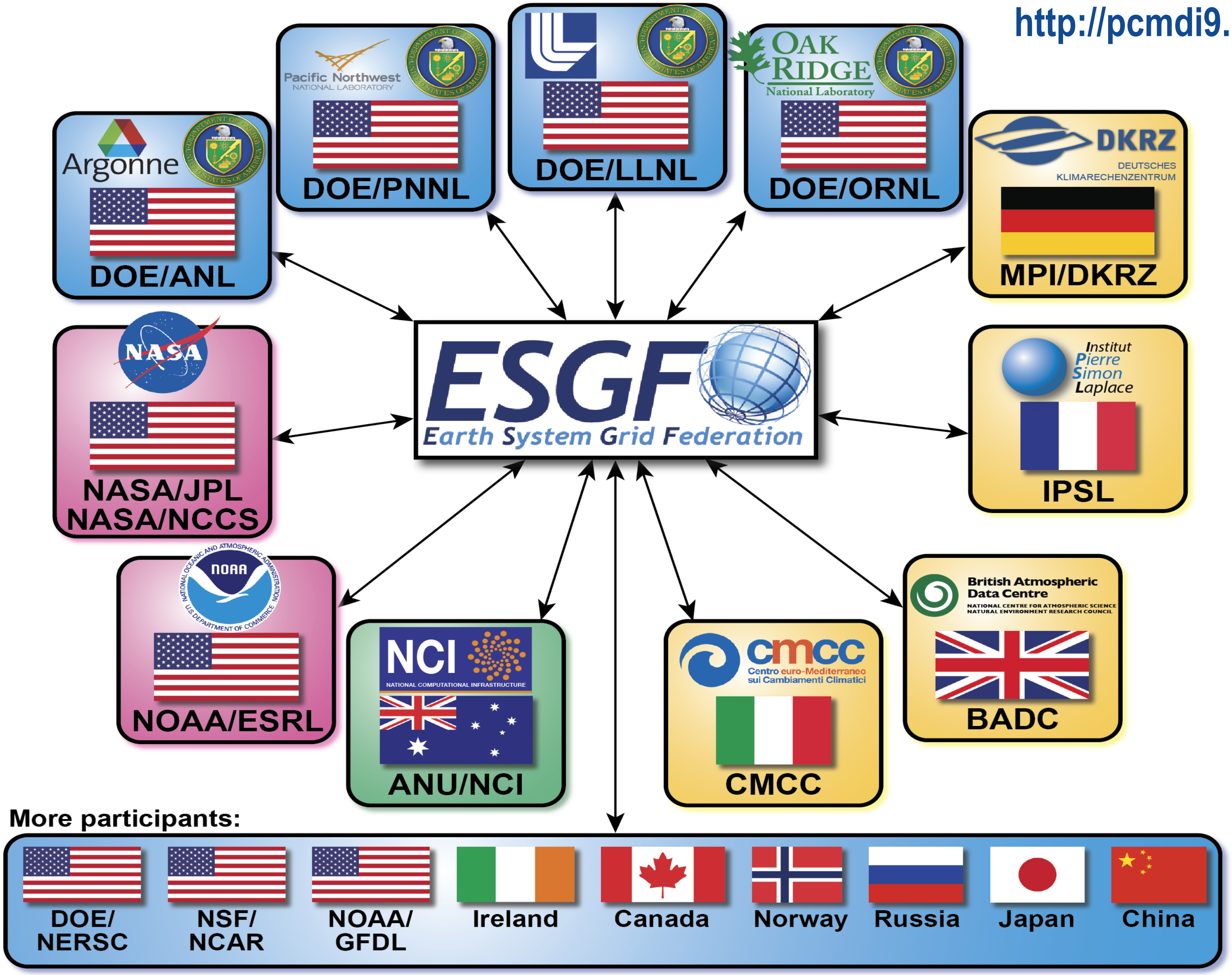
- **Publishing data** to an ESGF portal performs QC Level 1 (QCL1) check
  - QCL1 data are visible to users and are indentified as QCL1 on the UI
- DKRZ (MPI) **quality control code** is run on data to perform QC Level 2 (QCL2) check
  - QCL2 data are visible to users and are indentified as QCL2 on the UI
  - **Statistical quality control** – automatically identify data unusual enough to need further inspection
- **Visual inspections** are performed for inconsistencies and metadata correctness at QC Level 3 (QCL3) check
  - QCL3 data are visible to users and are indentified as QCL3 on the UI
  - **Digital Object Identifiers (DOIs)** are given to data sets that pass the QCL3 check

ESGF data holdings (~2 PB)

- Phases 3 and 5 of the Coupled Model Intercomparison Project (CMIP3 and CMIP5)
- Coordiated Regional climate Downscaling Experiment (CORDEX)
- Climate Science for a Sustainable Energy Future (CSSEF)
- European Union Cloud Intercomparison, Process Study & Evaluation Project (EUCLIPSE)
- Geo-engineering Model Intercomparison Project (GeoMIP)
- Land-Use and Climate, Identification of robust impacts (LUCID)
- Paleoclimate Modeling Intercomparison Project (PMIP)
- Transpose-Atmospheric Model Intercomparison Project (TAMIP)
- Clouds and Cryosphere (cloud-cryo)
- Observational products more accessible for coupled model intercomparison (obs4MIPs)
- Reanalysis for the coupled model intercomparison (ANA4MIPs)
- Dynamical Core Model Intercomparison Project (DCMIP)
- Community Climate System Model (CCSM)
- Parallel Ocean Program (POP)
- North American Regional Climate Change Assessment Program (NARCCAP)
- Carbon Land Model Intercomparison Project (C-LAMP)
- Atmospheric Infrared Sounder (AIS)
- Microwave Limb Sounder (MLS)

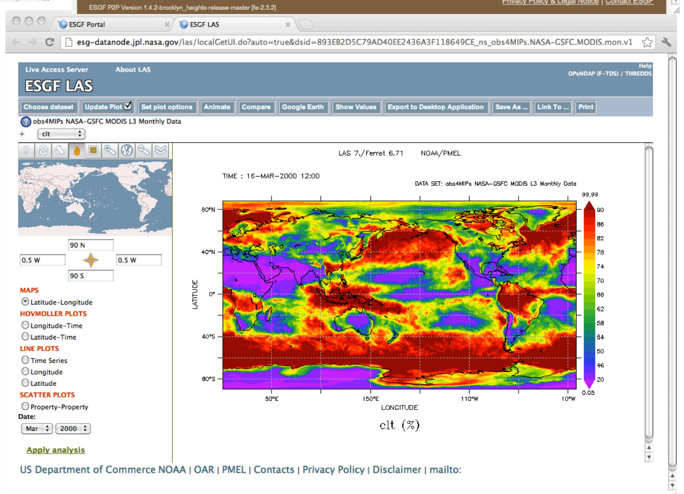
ESGF is more than CMIP: federated and integrated data from multiple sources

http://pcmdi9.llnl.gov/



†Additional participants could not be illustrated in this figure.

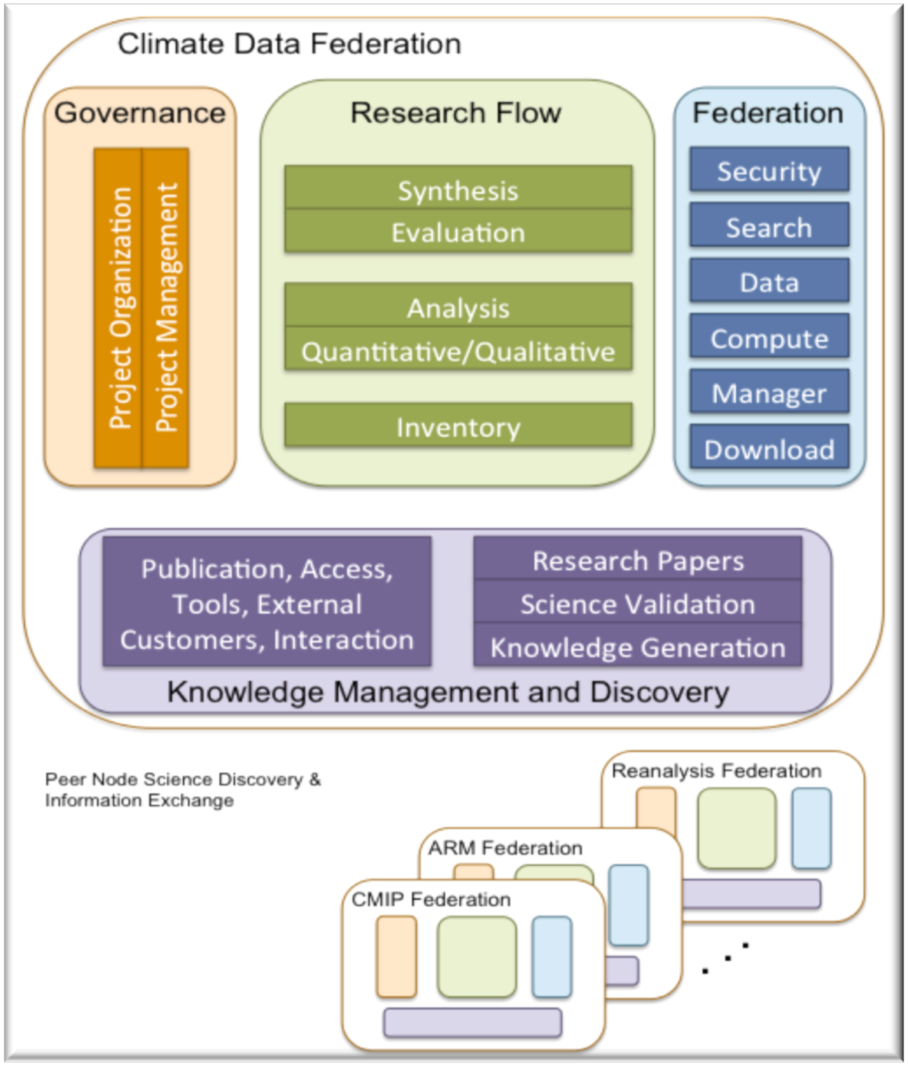
Example ESGF web portal



http://pcmdi9.llnl.gov/

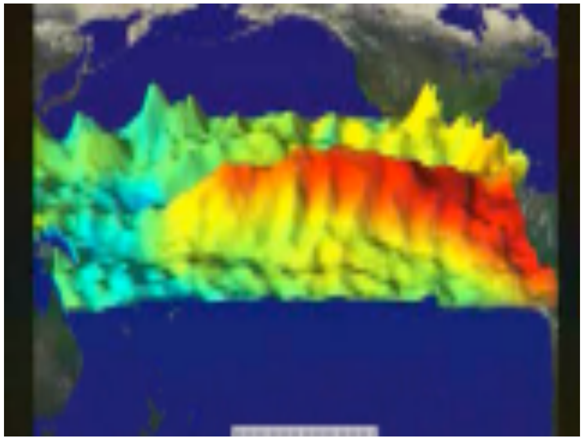
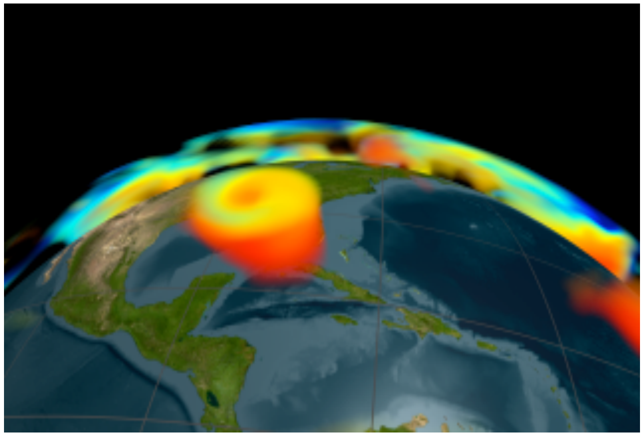
ESGF software system integrates data federation services

- NetCDF Climate and Forecast (CF) Metadata Convention
  - (LibCF)
  - Mosaic
- Climate Model Output Rewriter 2 (CMOR-2)
- Regriders: GRIDSPEC, SCRIP, & ESMF
- 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
- Security
- Product Services
  - Live Access Server, UV-CDAT



Advanced analytics, informatics, and visualization for scientists

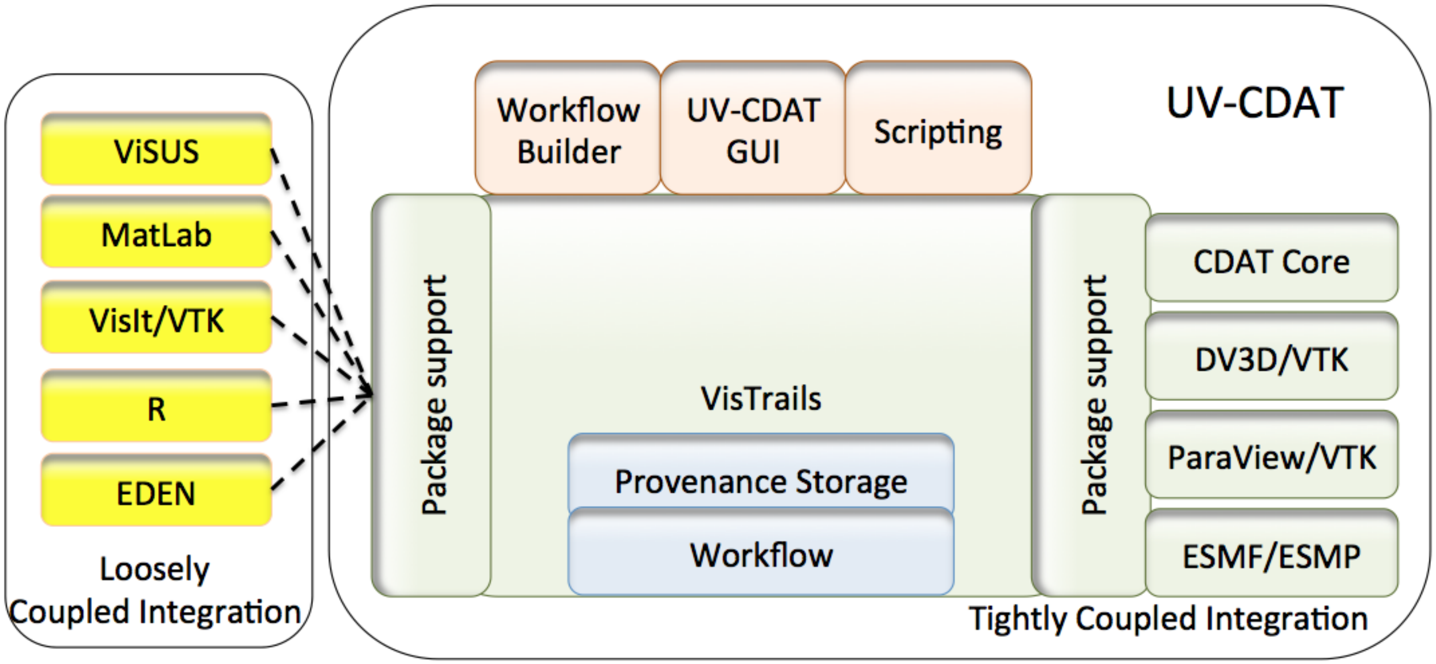
- Analysis and visualization is a key aspect of scientific analysis and discovery
- Advanced interactive visualization is rarely used by scientists
- Interfaces too complex, pickup too costly
- Interactive climate visualization requires:
  - Intuitive interfaces
  - Seamless integration with high performance analysis workbenches
  - Parallel streaming visualization pipelines

Background and introduction

http://uv-cdat.org/

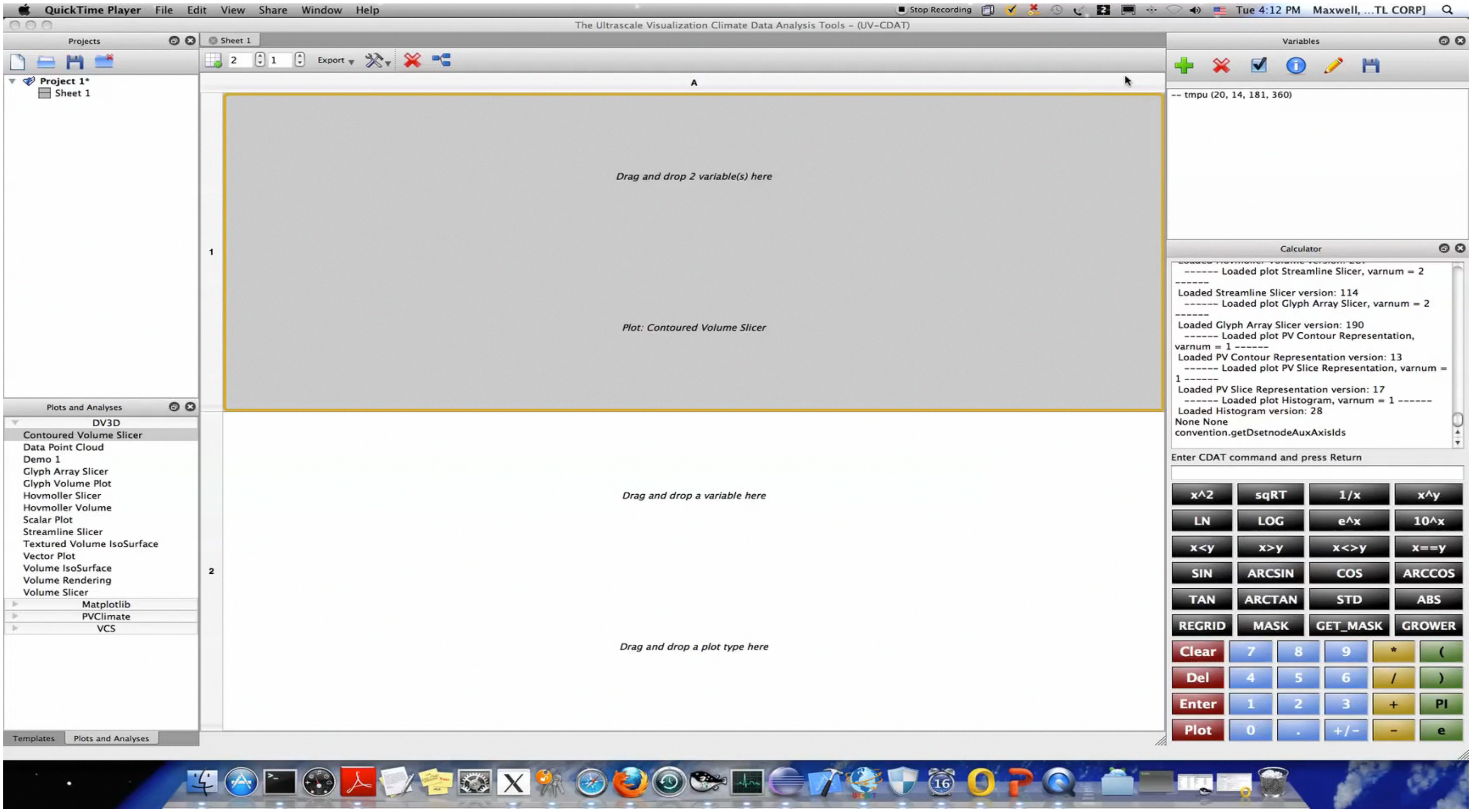
- **What is UV-CDAT:**
  - ❑ **A seamless environment for open-source data analysis and visualization packages**



- **What is UV-CDAT purpose:**
  - ❑ **Bring together robust tools for climate data processing**
  - ❑ **Integration heterogeneous data sources (e.g., simulations, observation, re-analysis)**
  - ❑ **Local and remote data access and visualization**
  - ❑ **Reproducibility**

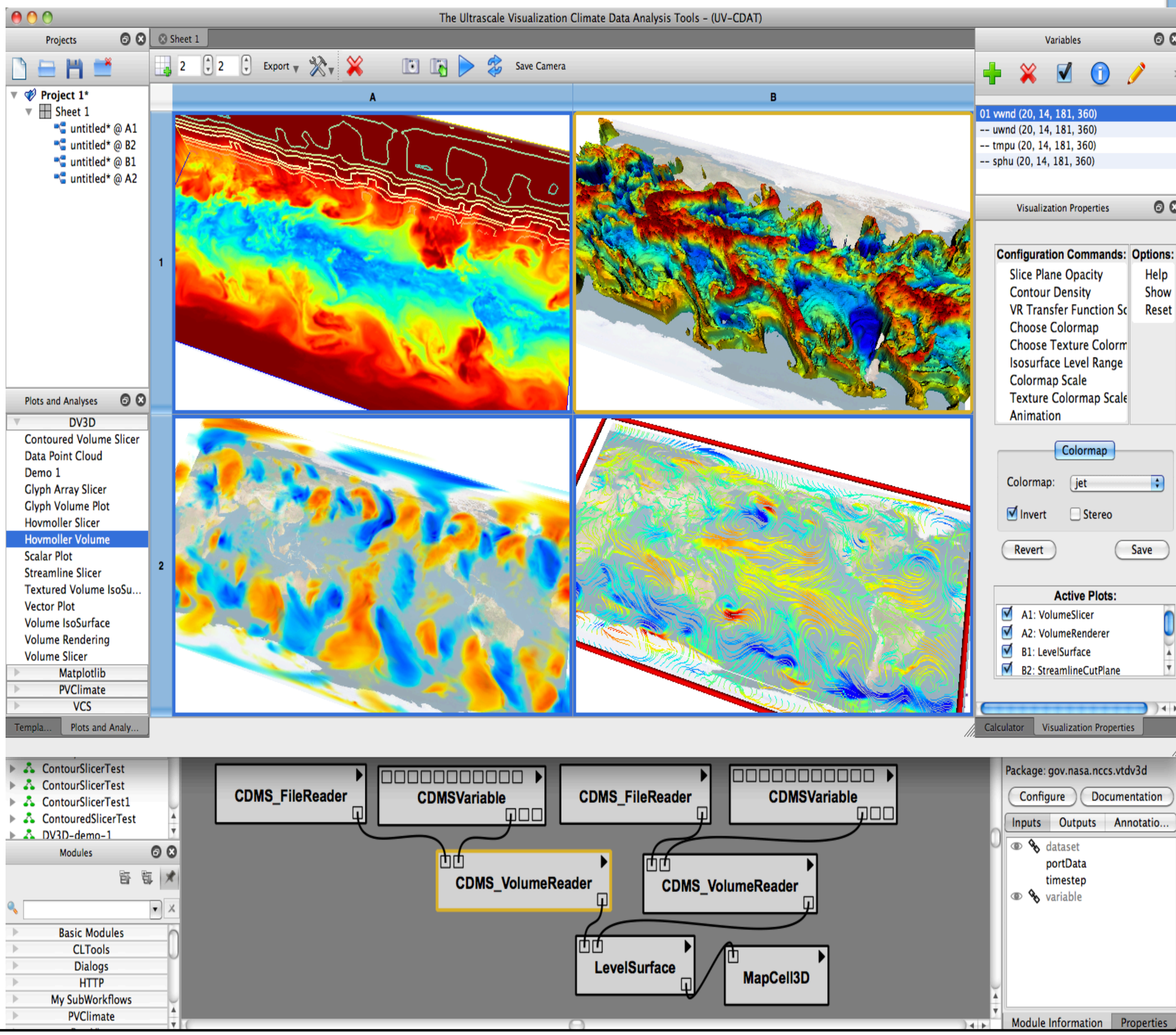
Interactive visualization and analysis

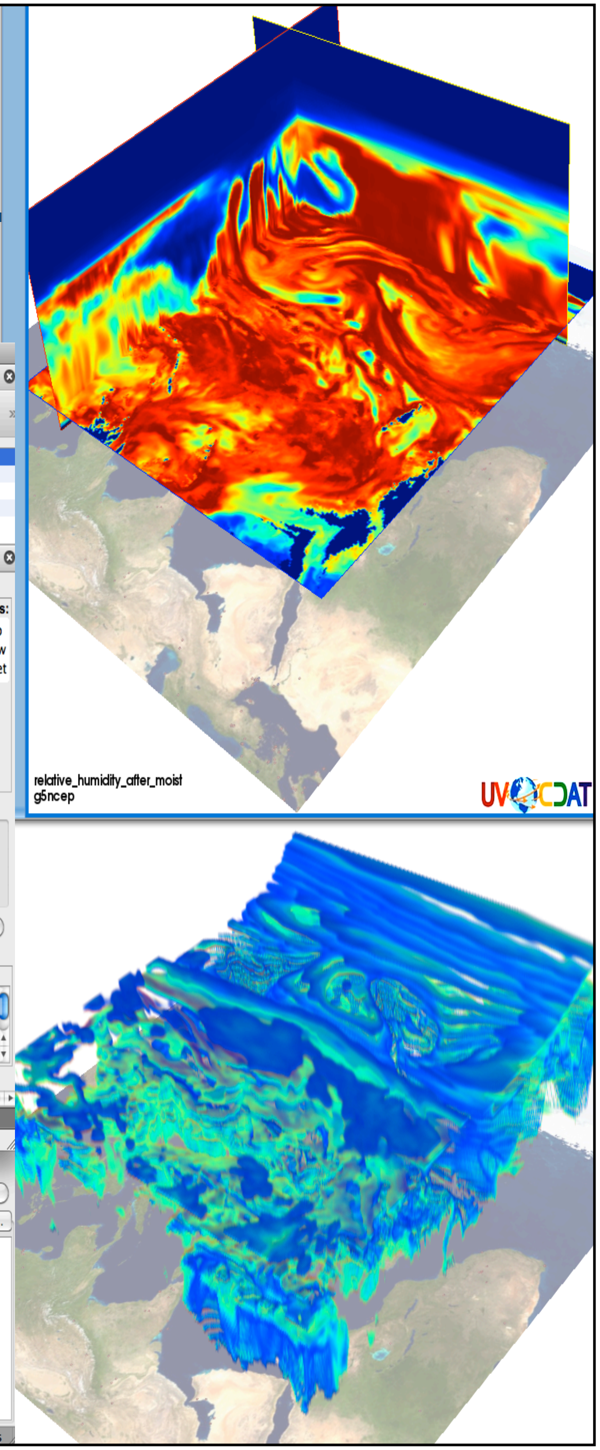
- Drag-and-drop variable and plots to create visualizations.
- Each plot has many user-friendly configuration options.



DV3D in UV-CDAT GUI

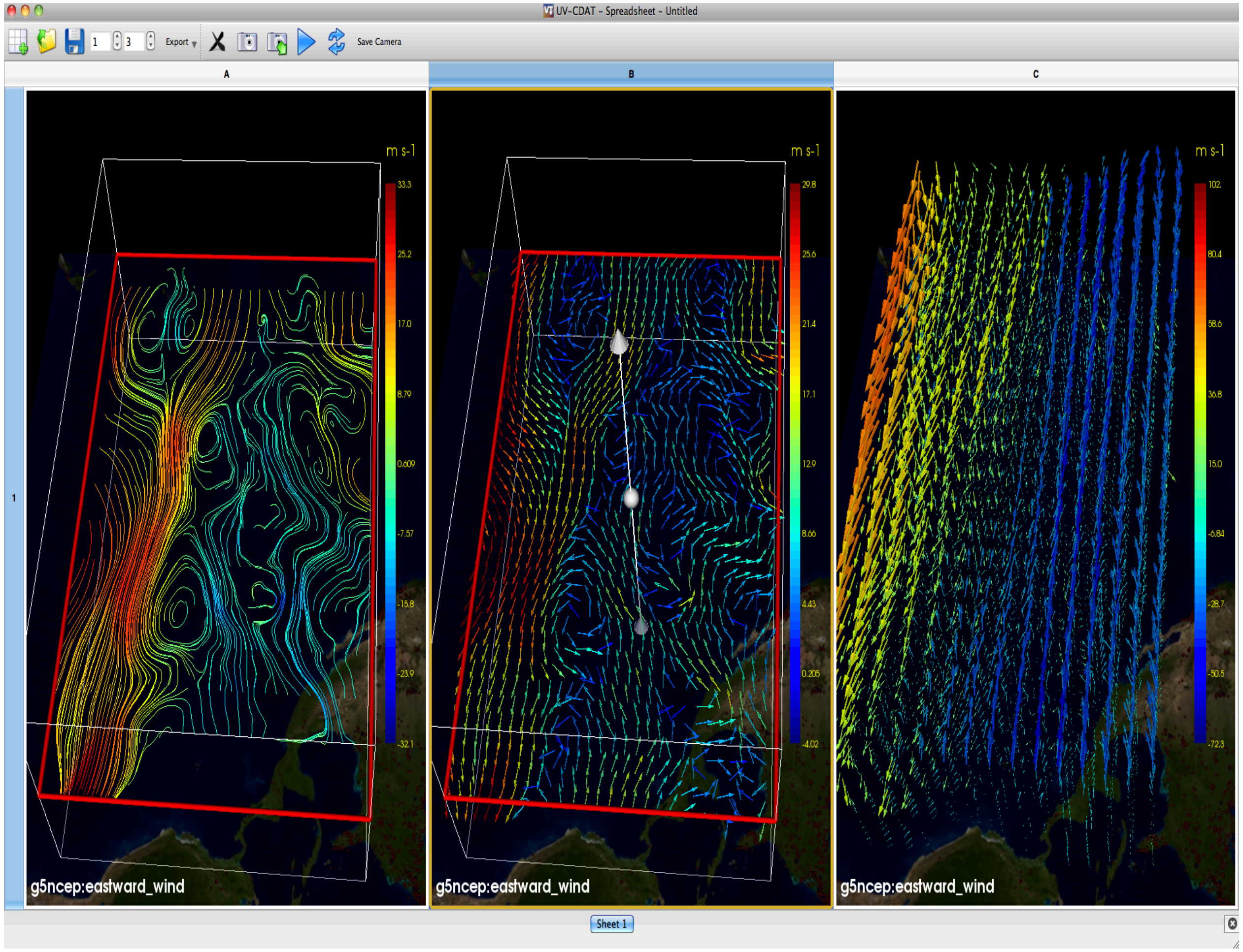
- Tightly integrated into the UVCDAT GUI.
- Inherits the Vistrails workflow and provenance support.





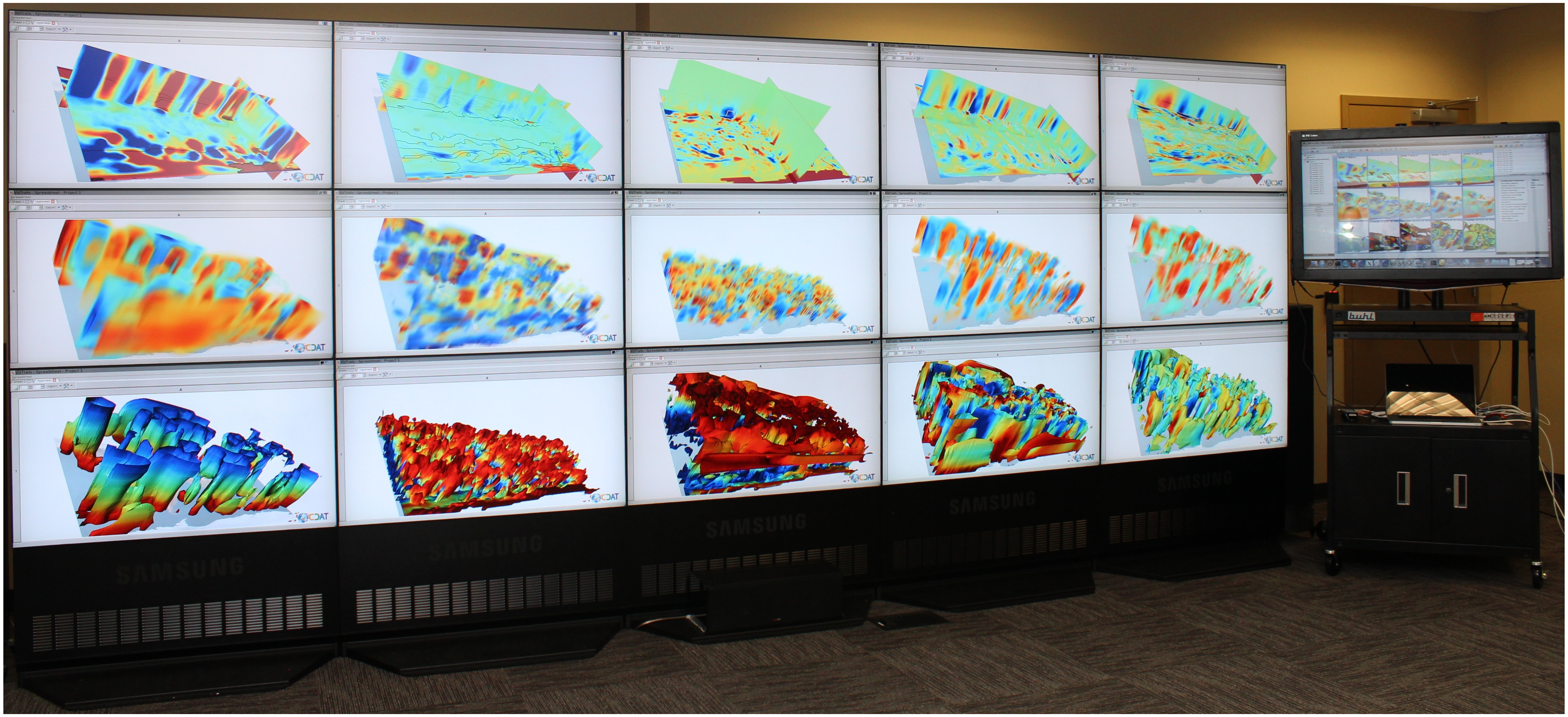
Vector plots

- Facilitates the visualization of 3D vector fields
- Utilizes streamlines on slices, glyphs on slices, or glyph volumes



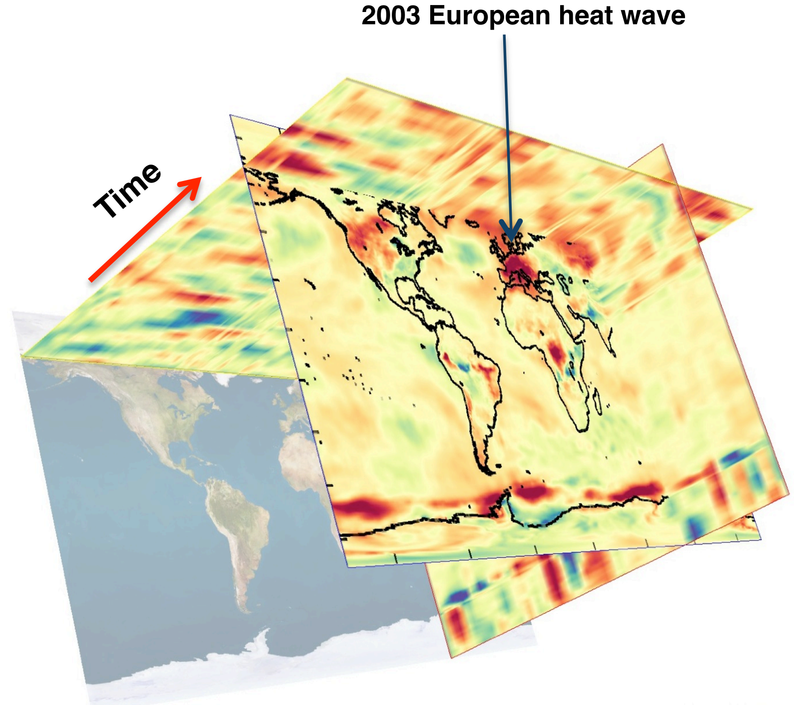
Interactive hyperwall visualization

- Uses parallelism to address data complexity
- UVCDAT runs on each display node (full-res 1-cell hyperwall display)
- UVCDAT runs on control node (low-res 15-cell touchscreen display)
- Control node interactions broadcast to all hyperwall nodes



Using UV-CDAT's 2D and 3D Capabilities to Explore Explore Time Series Data

- Demo using DV3D to examine 2-meter temperature from MERRA reanalysis
  - Use of a "3D Hovmöller" to explore anomalies
  - Basic attribution of extreme heat waves
  - Use of 250 mb meridional wind anomaly to identify stationary Rossby Waves
  - Identification of possible new planetary wave
- Demo of 3D slicer to examine Hurricane Sandy (October 2012)



Spatio-temporal pipeline: UV-CDAT use case 1

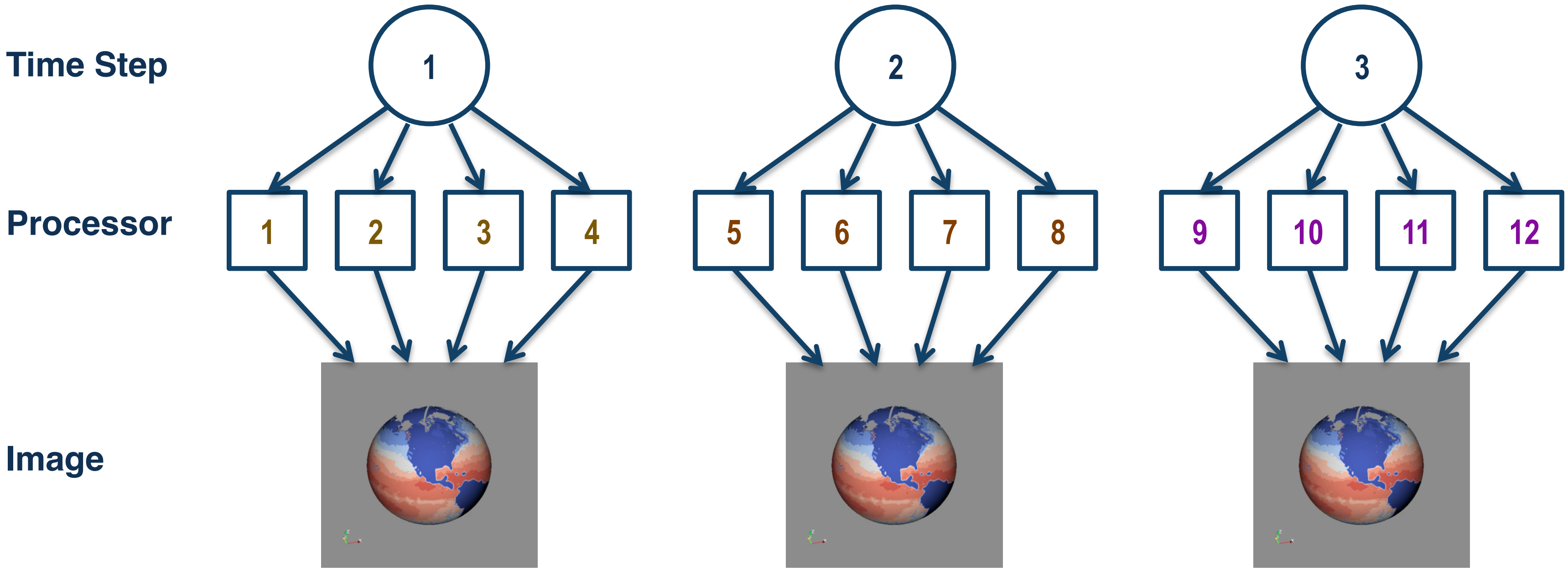
Use Case 1: High spatial resolution, high temporal resolution, image sequence production

Problem

Large datasets exist with many timesteps and high temporal resolution. UV-CDAT must be capable of handling these datasets. Existing tools do not support high temporal resolution well.

Solution

Added capability within UV-CDAT ParaView to partition within time to allow for multiple timesteps to be processed in parallel. Processors are divided into “time compartments”, and each file is processed by a time compartment.



Use Case 1 performance results: Mustang tests

Number of Timesteps	Number of Processes (P)	Time Compartment = P (seconds)	Time Compartment = 8 (seconds)
2	16	46.96	21.76
4	32	81.84	21.47
8	64	159.77	21.16
16	128	235.61	26.85
32	256	1,103.00	23.13
64	512	2,365.89	25.02
128	1024	8,128.92 (~2 hrs)	30.15
256	**2048**	**28,862.55 (~8 hrs)**	**62.83**

- Measured on Mustang supercomputer, 8 cores per node
- Each time step is 1.4 GB
- Panasas parallel file system
- Testing having all processors read each time step versus having eight processors read each time step

Spatio-temporal pipeline: UV-CDAT use case 2

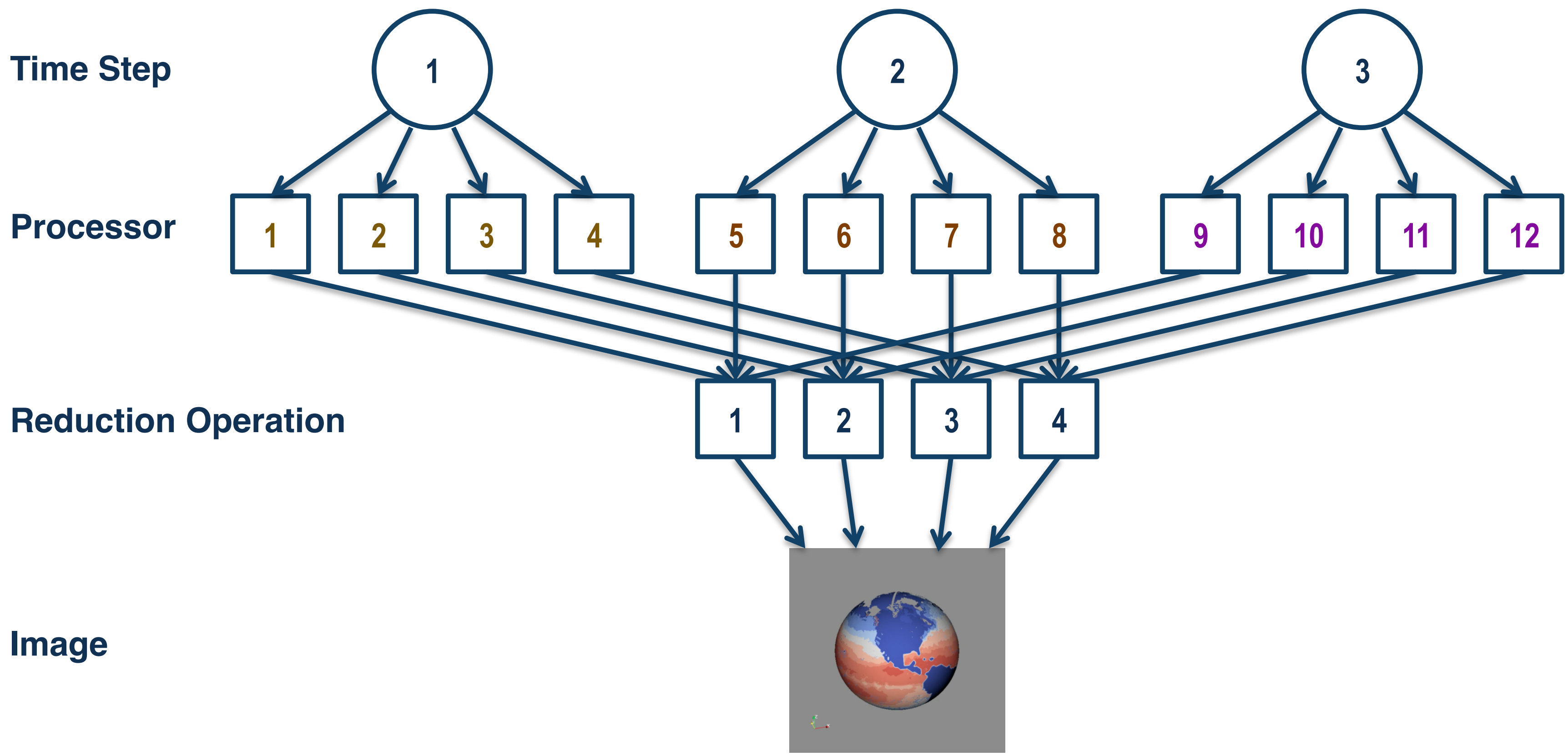
Use Case 2: High spatial resolution, high temporal resolution, time average

Problem

Multiple timesteps need to be averaged together to produce a data product based on the results.

Solution

Added capability within UVCDAT ParaView to take multiple timesteps and compute various statistics (average, min, max, standard deviation) using the spatio-temporal pipeline.



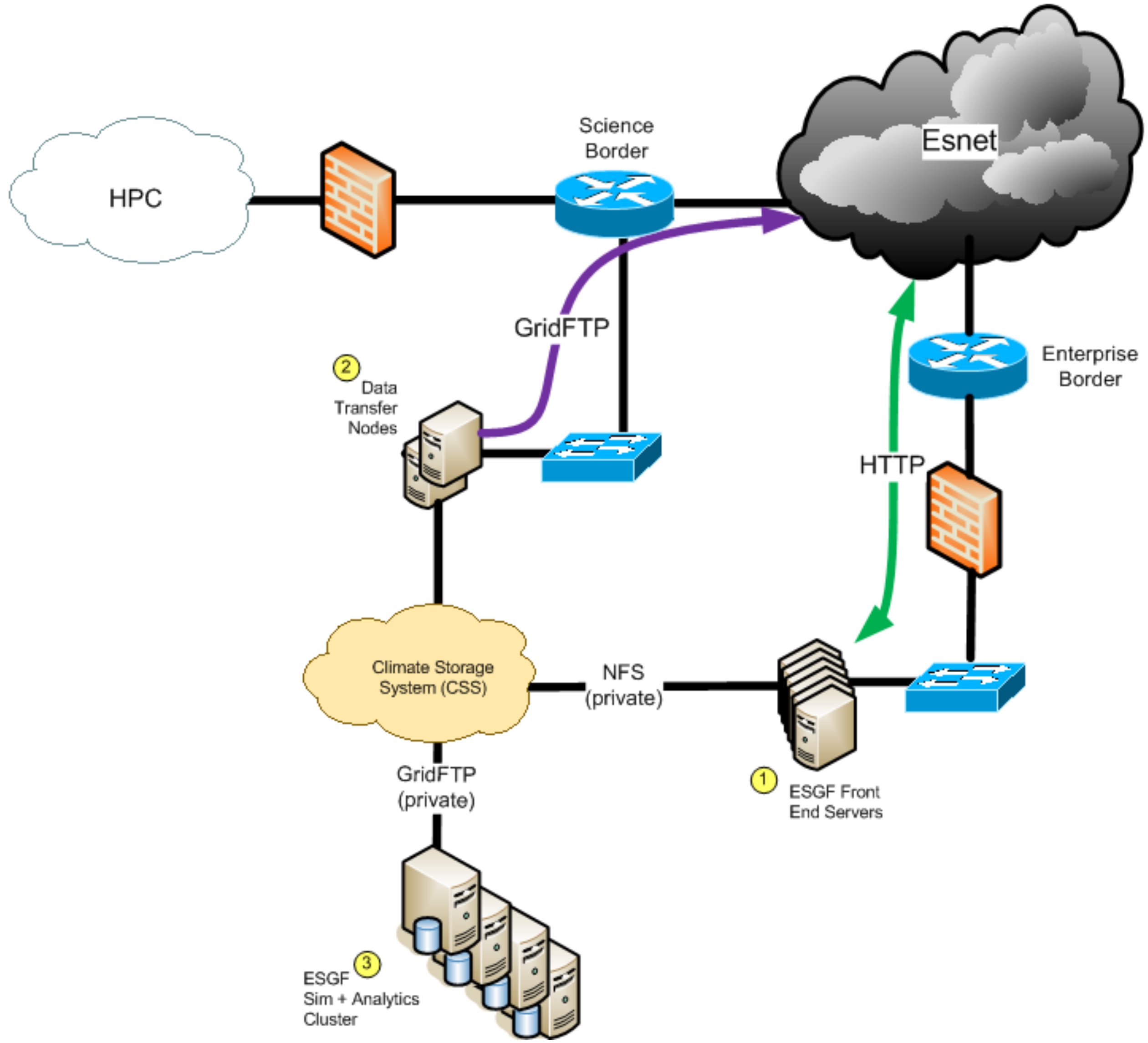
Use Case 2 performance results: Hopper tests

Time Compartment Size	Total Time (seconds)
1	145
2	278
12	**93**
48	151
96	244
240	525
480	1204

- Measured on Hopper supercomputer
- 480 cores, 20 nodes
- Analysis of Michael Wehner's climate data
- 324 timesteps, total data size is 20 GB
- Calculate yearly statistics from monthly data
    - Min, max, average, standard deviation
- Lustre parallel file system

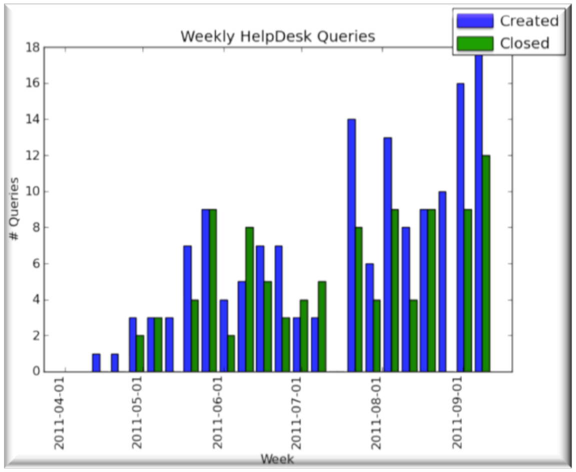
ESGF/UV-CDAT integrated with the hardware and network

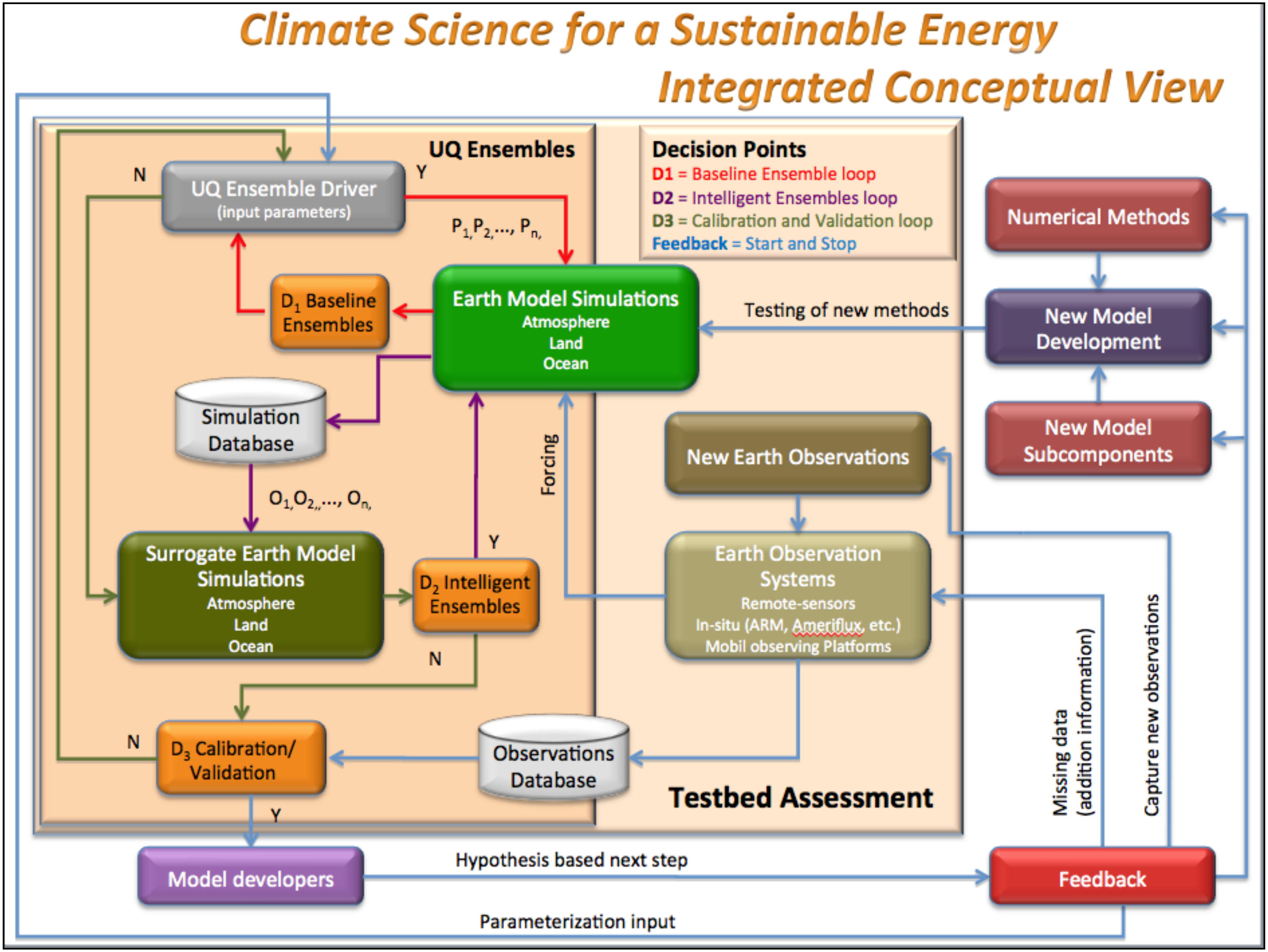
1. Users communicate with ESGF front-end servers via HTTP
2. Large data sets are made available to users directly from the Climate Storage System (CSS) via vsftp and GridFTP
3. Through UV-CDAT, ESGF will perform analysis of raw data if requested by users through the front-end servers to the analysis (hadoop) cluster



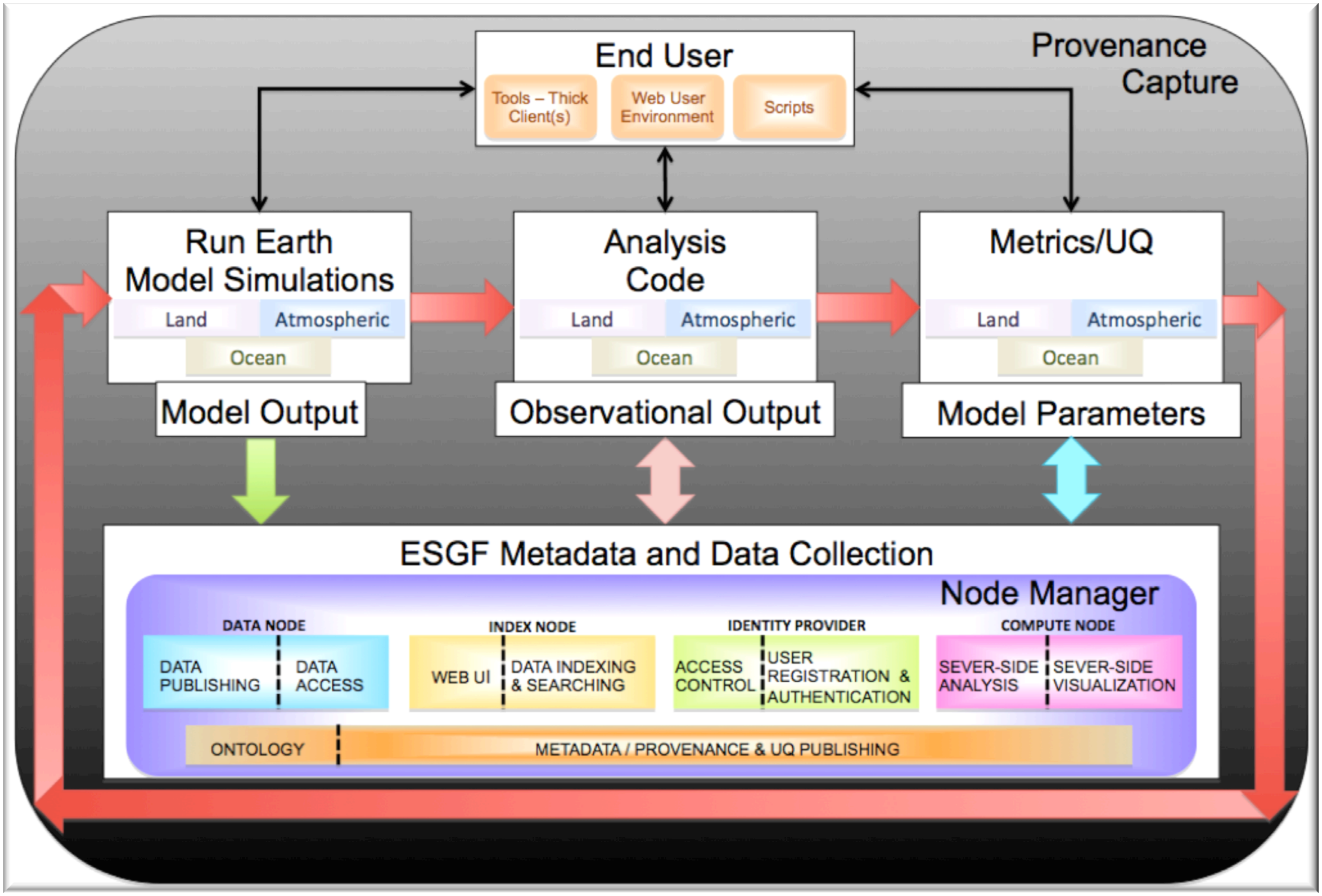
ESGF's and UV-CDAT multiple collaborations

■ ■ ■




Climate Science for a Sustainable Energy
Integrated Conceptual View
UQ Ensembles
UQ Ensemble Driver
(input parameters)
N
Y
P1, P2,..., Pn,
Decision Points
D1 = Baseline Ensemble loop
D2 = Intelligent Ensembles loop
D3 = Calibration and Validation loop
Feedback = Start and Stop
D1 Baseline Ensembles
Earth Model Simulations
Atmosphere
Land
Ocean
Testing of new methods
Numerical Methods
New Model Development
New Model Subcomponents
Simulation Database
Forcing
New Earth Observations
O1, O2,..., On,
Y
Surrogate Earth Model Simulations
Atmosphere
Land
Ocean
D2 Intelligent Ensembles
Earth Observation Systems
Remote-sensors
In-situ (ARM, Ameriflux, etc.)
Mobil observing Platforms
N
N
D3 Calibration/ Validation
Observations Database
Testbed Assessment
Missing data
(addition information)
Capture new observations
Y
Model developers
Hypothesis based next step
Feedback
Parameterization input

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



Questions and discussion