ACME – Accelerated Climate Modeling For Energy

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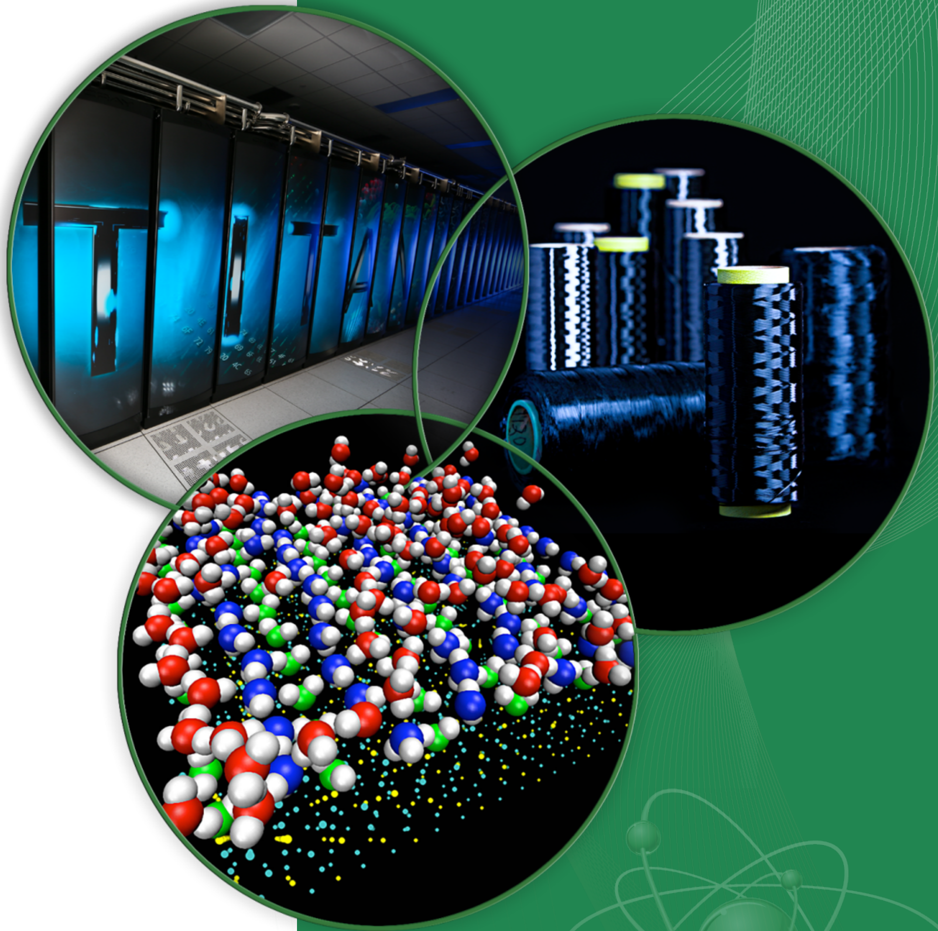

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OAK RIDGE National Laboratory | OAK RIDGE LEADERSHIP COMPUTING FACILITY

What is ACME?

- ***Multi-institutional, multi-disciplined, BER funded climate science effort***
- ***Proposal accepted June 1 for 3 years***
- ***Mission:***

  Build and test a next-generation earth modeling system that can be run on future generations of exascale computing systems at Office of Science computing facilities

What is ACME?

- ***Science Drivers:***
  - How do the hydrological cycle and water resources interact with the climate system on local to global scales?
  - How do biogeochemical cycles interact with global climate change?
  - How do rapid changes in cryospheric systems interact with the climate system?
- ***Science Needs:***
  - Support of wide range of model runs and workflow types
  - Capture of model runs, settings and data during development
  - Quickly evaluate and validate model behavior

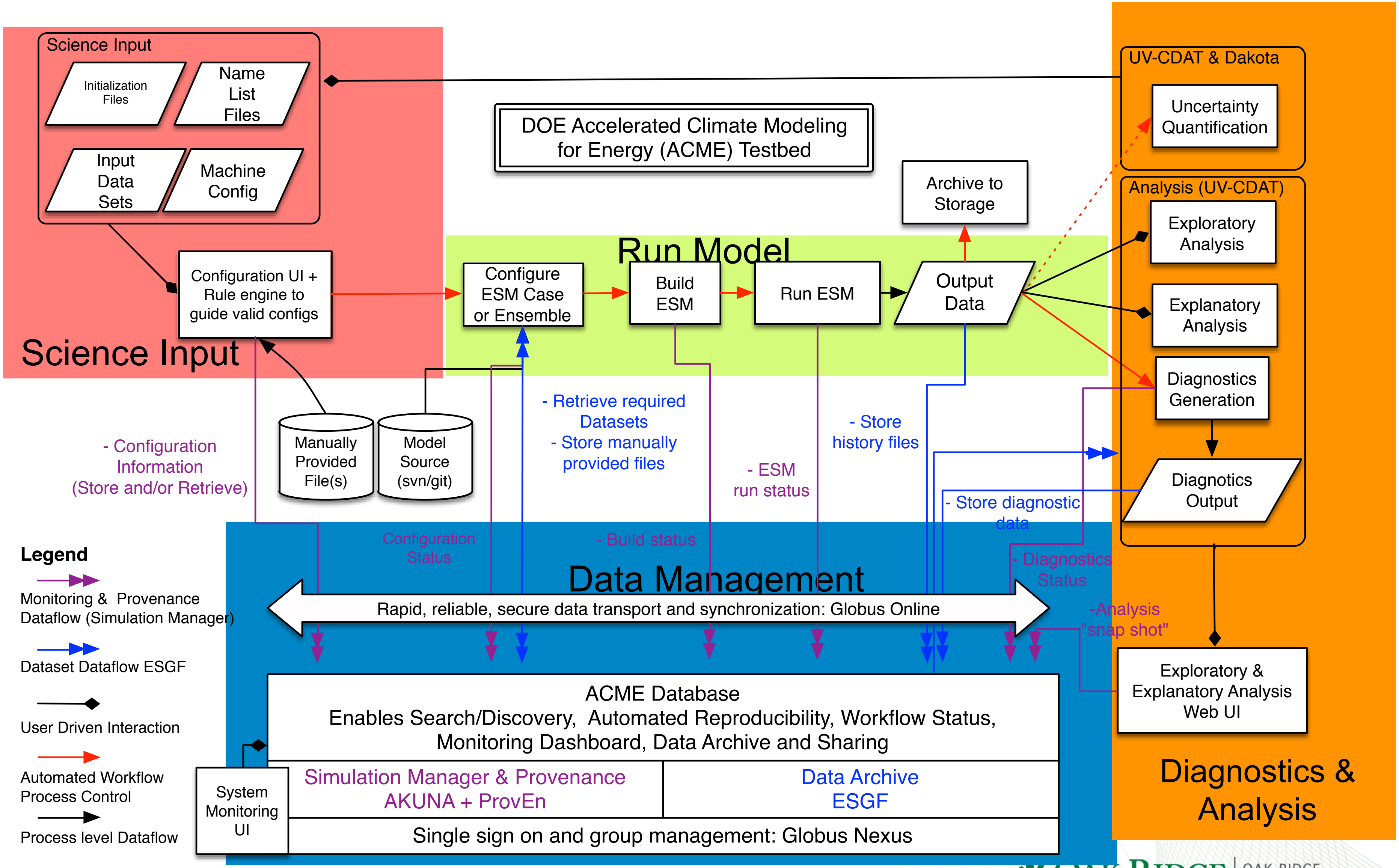
ACME Solutions

Science Needs	Solution
Support of wide range of model runs and workflow types across the project	Define use cases: 1) Model Development (DEV); (2) Exploratory Model Runs (EXP); (3) Production Model Runs (PROD) Hi-res and low-res
Capture and record suites of runs and their settings during model development	Automated provenance and archiving throughout the life cycle of the model
Quickly evaluate coupled model behavior	Advanced diagnostics of the coupled system within one software system

Major challenges for the ACME end-to-end system

Challenges	Description
Installation	Software must adapted to multiple hardware platforms and operating systems located throughout the ACME
Heterogeneous Data Sets	The same infrastructure must also allow scientists to access and compare data sets from multiple sources, including from observational satellite and instrument sources
Analysis, Diagnostics, and Visualizations	The generation of new and improved analysis, diagnostics, and visualization techniques for the better model development and evaluation
Server-side and In Situ Computing	Server-side and in situ computation is necessary as the increase in data size and complexity of algorithms lead to data-intensive, compute-intensive challenges for ACME diagnostics, UQ, analysis, model metrics, and visualization

End-to-end workflow



Science Input

Initialization Files

Name List Files

Input Data Sets

Machine Config

Configuration UI + Rule engine to guide valid configs

Science Input

DOE Accelerated Climate Modeling for Energy (ACME) Testbed

Run Model

Configure ESM Case or Ensemble

Build ESM

Run ESM

Output Data

Archive to Storage

Manually Provided File(s)

Model Source (svn/git)

- Configuration Information (Store and/or Retrieve)

- Retrieve required Datasets
- Store manually provided files

- ESM run status

- Store history files

- Store diagnostic data

Configuration Status

- Build status

- Diagnostics Status

-Analysis "snap shot"

UV-CDAT & Dakota

Uncertainty Quantification

Analysis (UV-CDAT)

Exploratory Analysis

Explanatory Analysis

Diagnostics Generation

Diagnotics Output

Exploratory & Explanatory Analysis Web UI

Diagnostics & Analysis

Data Management

Rapid, reliable, secure data transport and synchronization: Globus Online

ACME Database
Enables Search/Discovery, Automated Reproducibility, Workflow Status, Monitoring Dashboard, Data Archive and Sharing

Simulation Manager & Provenance AKUNA + ProvEn	Data Archive ESGF

Single sign on and group management: Globus Nexus

System Monitoring UI

Legend

Monitoring & Provenance Dataflow (Simulation Manager)

Dataset Dataflow ESGF

User Driven Interaction

Automated Workflow Process Control

Process level Dataflow

Science Input & Run Model – Streamlining CESM

- Model development tasks (configure, interpolation, run, build) are tedious and time-consuming
- ACME partners developers and scientists to define and iteratively implement in (semi-)automated end-to-end science workflow. Ideally reduces:
  - Scientist effort to setup/run an experiment
  - Time to solution by automating running of CESM
  - Queue wait times
  - Delays of human intervention
- Implement so automation “just happens” or can be used as helper scripts by hand

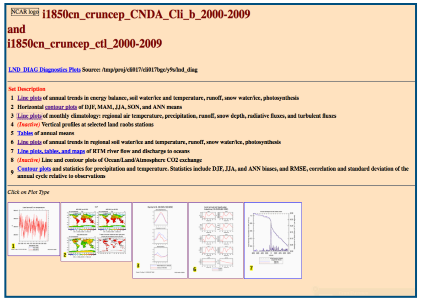
Science Input & Run Model – Workflow automation

- Workflow progress on compute resources is reported back by each workflow component via AMQP messaging broker
  - Leverage existing DOE technology to consume messages (e.g. Akuna from PNNL)
- Create central place to see progress of simulations
  - Current progress (e.g. 23 / 50 years)
  - Current status of data (simulation progress, HPSS, etc)
- Direct links to archives and diags framework

Diagnostics and Analysis

- Diagnostics
  - Used to quickly evaluate models and validate their results
  - Traditional CESM NCL scripts from NCAR produce static HTML and plots (gif, jpg, etc)

Diagnostics Home (Plot types of realms)



NCAR logo **i1850cn_cruncep_CNDA_Cli_b_2000-2009**
and
i1850cn_cruncep_ctl_2000-2009

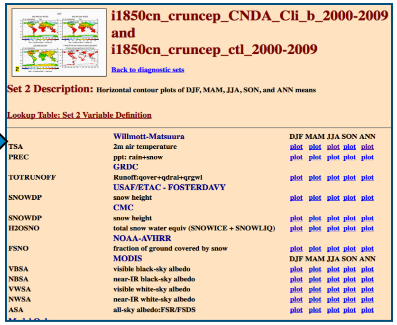
LND_DIAG Diagnostics Plots Source: /tmp/proj/cli017/cli017bgc/y9s/lnd_diag

Set Description

1 Line plots of annual trends in energy balance, soil water/ice and temperature, runoff, snow water/ice, photosynthesis
2 Horizontal contour plots of DJF, MAM, JJA, SON, and ANN means
3 Line plots of monthly climatology: regional air temperature, precipitation, runoff, snow depth, radiative fluxes, and turbulent fluxes
4 *(Inactive)* Vertical profiles at selected land raobs stations
5 Tables of annual means
6 Line plots of annual trends in regional soil water/ice and temperature, runoff, snow water/ice, photosynthesis
7 Line plots, tables, and maps of RTM river flow and discharge to oceans
8 *(Inactive)* Line and contour plots of Ocean/Land/Atmosphere CO2 exchange
9 Contour plots and statistics for precipitation and temperature. Statistics include DJF, JJA, and ANN biases, and RMSE, correlation and standard deviation of the annual cycle relative to observations

Click on Plot Type

Variable List



i1850cn_cruncep_CNDA_Cli_b_2000-2009
and
i1850cn_cruncep_ctl_2000-2009

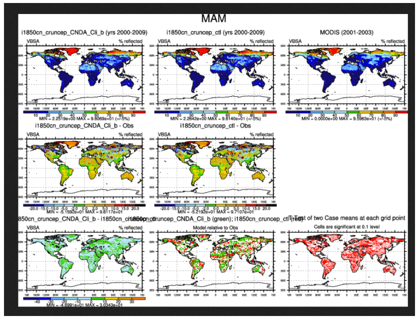
Back to diagnostic sets

Set 2 Description: Horizontal contour plots of DJF, MAM, JJA, SON, and ANN means

Lookup Table: Set 2 Variable Definition

	Willmott-Matsuura	DJF	MAM	JJA	SON	ANN
TSA	2m air temperature	plot	plot	plot	plot	plot
PREC	ppt: rain+snow	plot	plot	plot	plot	plot
	GRDC					
TOTRUNOFF	Runoff:qover+qdrai+qrgwl	plot	plot	plot	plot	plot
	USAF/ETAC - FOSTERDAVY					
SNOWDP	snow height	plot	plot	plot	plot	plot
	CMC					
SNOWDP	snow height	plot	plot	plot	plot	plot
H2OSNO	total snow water equiv (SNOWICE + SNOWLIQ)	plot	plot	plot	plot	plot
	NOAA-AVHRR					
FSNO	fraction of ground covered by snow	plot	plot	plot	plot	plot
	MODIS	DJF	MAM	JJA	SON	ANN
VBSA	visible black-sky albedo	plot	plot	plot	plot	plot
NBSA	near-IR black-sky albedo	plot	plot	plot	plot	plot
VWSA	visible white-sky albedo	plot	plot	plot	plot	plot
NWSA	near-IR white-sky albedo	plot	plot	plot	plot	plot
ASA	all-sky albedo:FSR/FSDS	plot	plot	plot	plot	plot

Plot

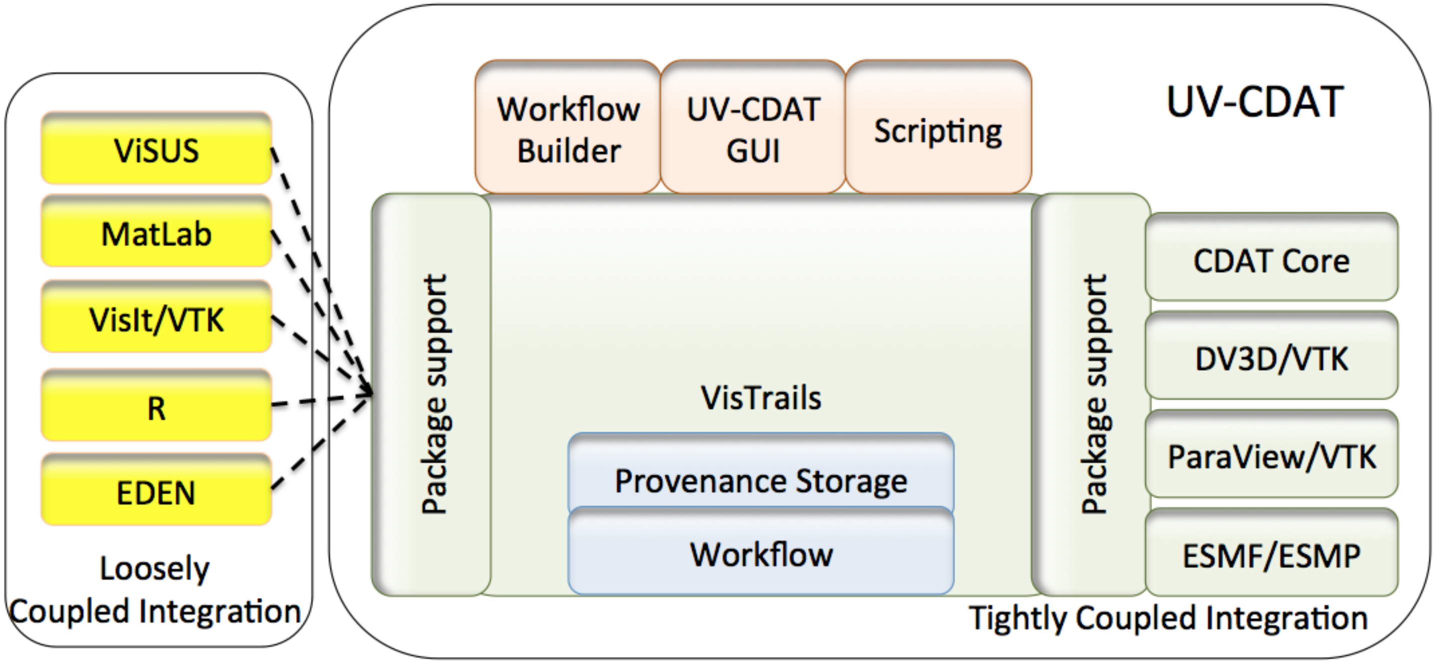


MAM
i1850cn_cruncep_CNDA_Cli_b (yrs 2000-2009)
i1850cn_cruncep_ctl (yrs 2000-2009)
MODIS (2001-2003)
VBSA
% reflected
MIN = 2.2519e+00 MAX = 9.8069e+01 (+/-5%)
MIN = 2.2642e+00 MAX = 9.8140e+01 (+/-5%)
MIN = 0.0000e+00 MAX = 9.5963e+01 (+/-5%)
i1850cn_cruncep_CNDA_Cli_b - Obs
i1850cn_cruncep_ctl - Obs
MIN = -5.1592e+01 MAX = 9.6117e+01
MIN = -5.2192e+01 MAX = 9.7107e+01
850cn_cruncep_CNDA_Cli_b - i1850cn_cruncep_ctl
i1850cn_cruncep_CNDA_Cli_b (green); i1850cn_cruncep_ctl (red)
Model relative to Obs
T-Test of two Case means at each grid point
Cells are significant at 0.1 level
MIN = -4.6991e+01 MAX = 3.0343e+01

  - Need a more scalable, dynamic and intuitive diags package so results can be ascertained and validated quickly

Diagnostics and Analysis - UVCDAT

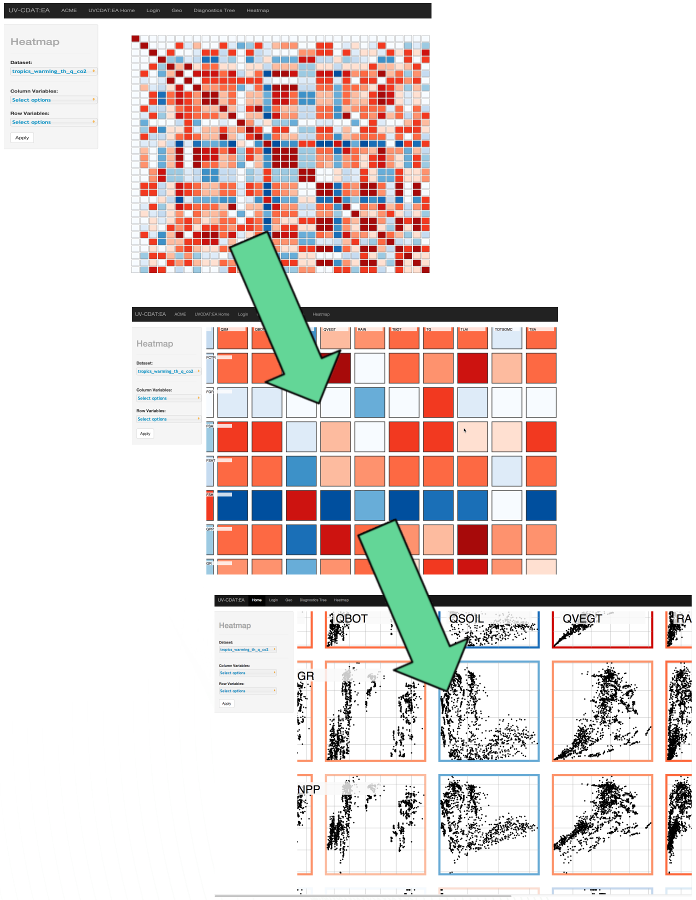
- What is UV-CDAT:
  - ❑ A seamless environment for open-source data analysis and visualization packages



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

Diagnostics and Analysis – Web-based Visual Analytics

- Attractive alternative to standalone, thick client
  - Democratizes advanced visual analytics capacities
  - Greater efficiencies through distributed architecture
  - Runs in a web browser (D3, django, jquery)
  - Supports social collaboration
  - Compatibility with UVCDAT
  - Multiple views developed so far:
    - Interactive geospatial-temporal view
    - Diagnostics Tree Viewer
    - Heatmap variable correlation



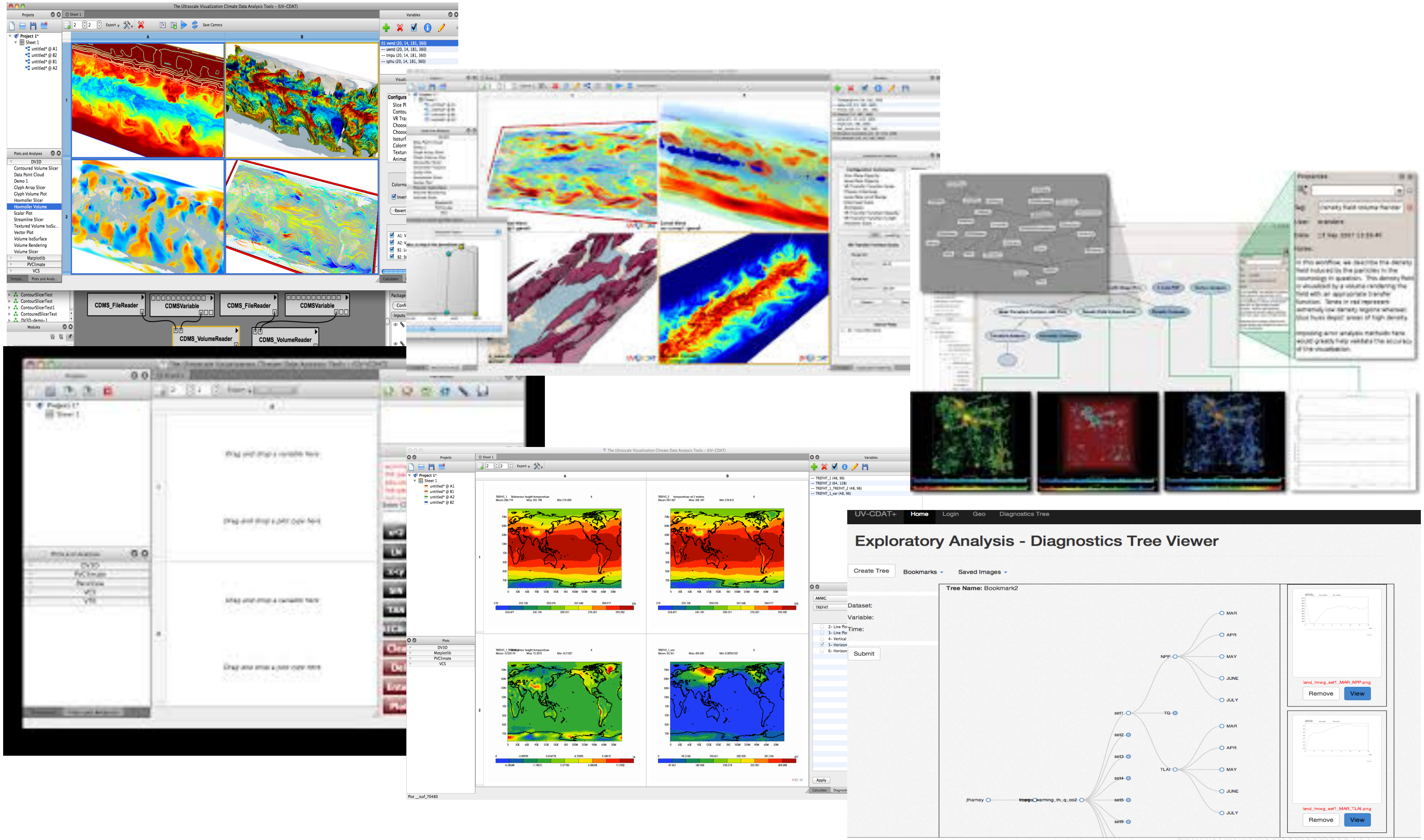
Dataset: tropics_warming_th_q_co2

Column Variables: Select options

Row Variables: Select options

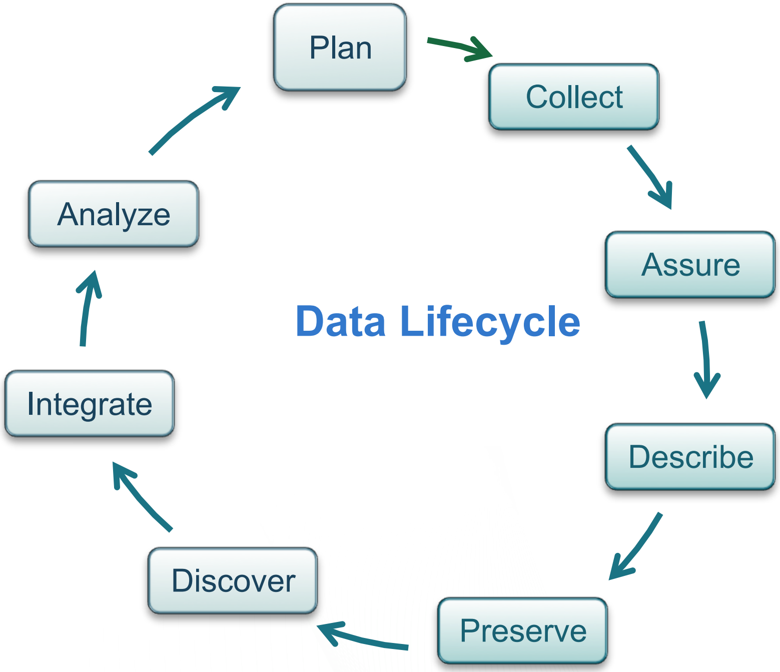
E.g. Web-based Heatmap Correlation

Diagnostics and Analysis – Examples



Data Management

- Output from completed models enter the ACME data management life cycle which supports:
  - Data Collection and Publication
  - Archiving and stewardship
  - Search and Discovery
  - Provenance Capture (i.e. Data/Algorithm reproducibility)
  - Fast/secure acquisition of data (downloads, transfers, etc)

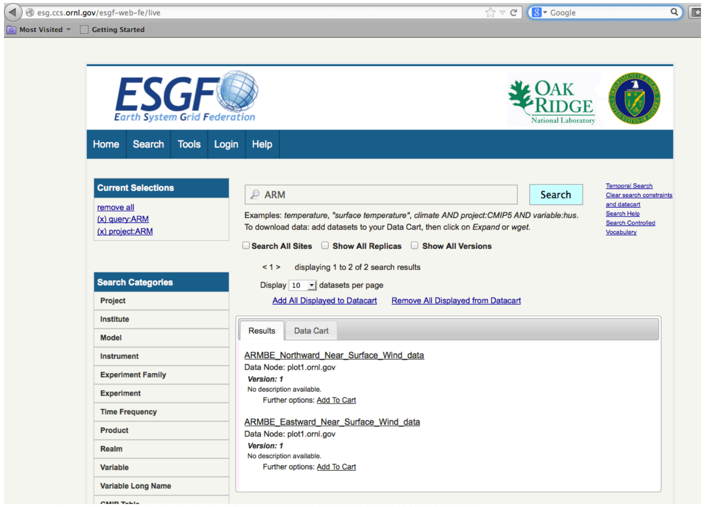


Data Management – Data Services

Earth System Grid Federation (ESGF)

- Distributed enterprise system that deploys software infrastructure for the management, collaboration, dissemination, and analysis of climate model output and observational data
- Over 30k published federation-wide datasets (over 1PB) in over 20 climate institutions worldwide
- Peer-to-Peer design for increased scalability and fault tolerance
- Solr search engine designed for optimal metadata cataloging and dataset retrieval
- Secure file access and group-based authorization services

ESGF
Earth System Grid Federation


esg.ccs.ornl.gov/esgf-web-fe/live
Google
Most Visited
Getting Started
ESGF Earth System Grid Federation
Oak Ridge National Laboratory
Home
Search
Tools
Login
Help
Search
Temporal Search
Clear search constraints and datacart
Search Help
Search Controlled Vocabulary
Results
Data Cart

Current Selections
remove all
(x) query:ARM
(x) project:ARM

ARM

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 10 datasets per page

Add All Displayed to Datacart Remove All Displayed from Datacart

Search Categories
Project
Institute
Model
Instrument
Experiment Family
Experiment
Time Frequency
Product
Realm
Variable
Variable Long Name
CMIP Table

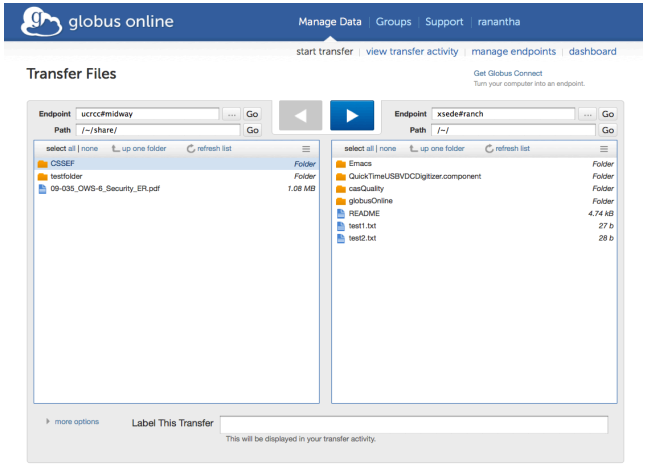
ARMBE_Northward_Near_Surface_Wind_data
Data Node: plot1.ornl.gov
Version: 1
No description available.
Further options: Add To Cart

ARMBE_Eastward_Near_Surface_Wind_data
Data Node: plot1.ornl.gov
Version: 1
No description available.
Further options: Add To Cart

Data Management – Data Services

Globus Online

- Reliable, secure, high-performance file transfer and synchronization
- “Fire-and-forget” transfers
- Automatic fault recovery
- Fully integrated with ESGF services
- Key technology in transferring large datasets (e.g. high resolution)



Transfer Files

Endpoint: ucrcc#midway
Path: /~/share/

CSSEF	Folder
testfolder	Folder
09-035_OWS-6_Security_ER.pdf	1.08 MB

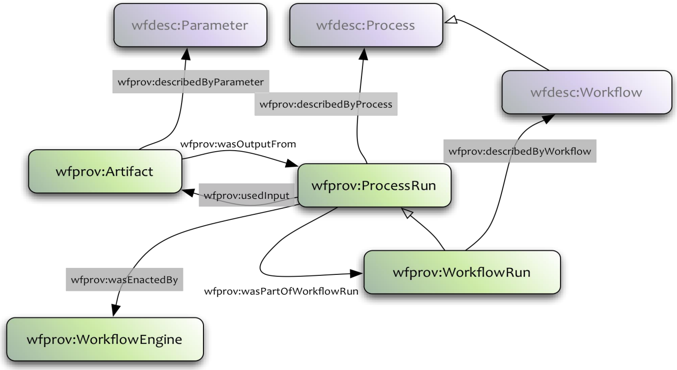
Endpoint: xsede#ranch
Path: /~/

Emacs	Folder
QuickTimeUSBVDCDigitizer.component	Folder
casQuality	Folder
globusOnline	Folder
README	4.74 kB
test1.txt	27 b
test2.txt	28 b

Label This Transfer

This will be displayed in your transfer activity.

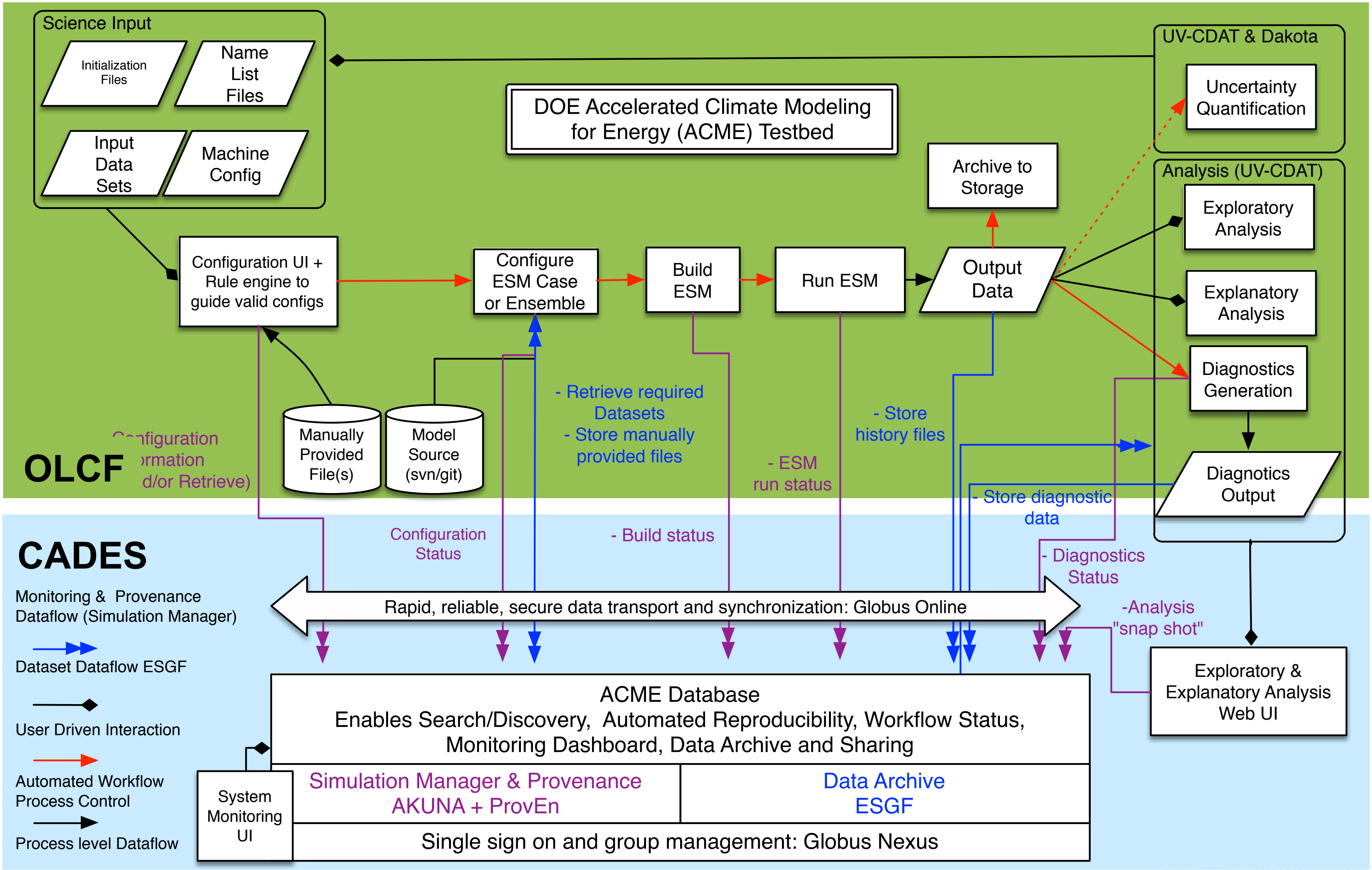
ESM Core Provenance Ontology



PROVEN

- Capture historical information from any native source necessary to describe the origin of the dataset
- Store this information in a cross-referenced form through the use of internationally recognized standards W3C, Dublin Core, CF
- Use this cross-referenced information to provide finished products to different kinds of consumers
- Will be integrated with ESGF in future release

End-to-end workflow and data infrastructure architecture



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OLCF

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CADES

Configuration Status

- Build status

- Diagnostics Status

-Analysis "snap shot"

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Exploratory & Explanatory Analysis Web UI

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Data Archive
ESGF

Single sign on and group management: Globus Nexus

System Monitoring UI

Monitoring & Provenance Dataflow (Simulation Manager)

Dataset Dataflow ESGF

User Driven Interaction

Automated Workflow Process Control

Process level Dataflow

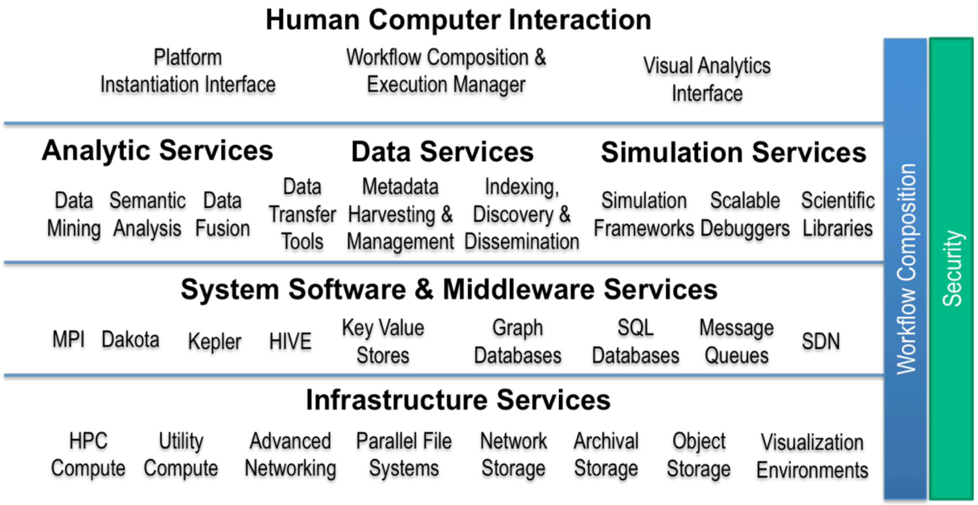
CADES

Compute & Data Environment for Science

CADES provides core compute and data services required by major science facilities, large projects, small teams, and single principal investigators

CADES is a cross-cutting center: it shares both data infrastructure and compute & data science expertise with and among many projects

A rich set of flexibly composable services coupled with experts in data science partnering with domain scientists on their challenges



Human Computer Interaction

Platform Instantiation Interface | Workflow Composition & Execution Manager | Visual Analytics Interface

Analytic Services: Data Mining | Semantic Analysis | Data Fusion

Data Services: Data Transfer Tools | Metadata Harvesting & Management | Indexing, Discovery & Dissemination

Simulation Services: Simulation Frameworks | Scalable Debuggers | Scientific Libraries

System Software & Middleware Services

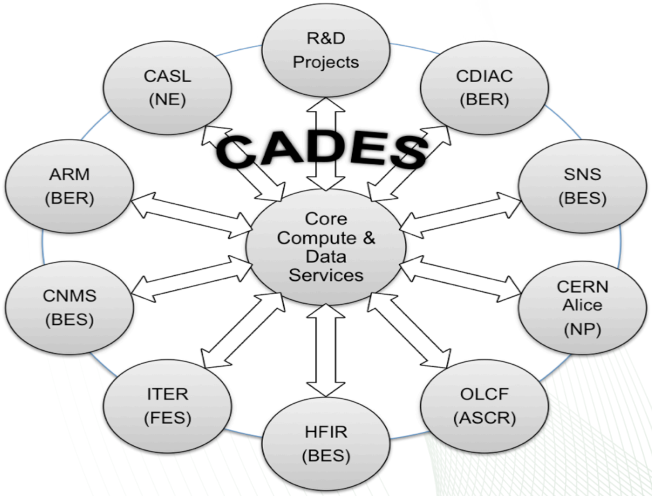
MPI | Dakota | Kepler | HIVE | Key Value Stores | Graph Databases | SQL Databases | Message Queues | SDN

Infrastructure Services

HPC Compute | Utility Compute | Advanced Networking | Parallel File Systems | Network Storage | Archival Storage | Object Storage | Visualization Environments

Workflow Composition

Security



CADES

Core Compute & Data Services

R&D Projects

CDIAC (BER)

SNS (BES)

CERN Alice (NP)

OLCF (ASCR)

HFIR (BES)

ITER (FES)

CNMS (BES)

ARM (BER)

CASL (NE)

Experiences and Lessons Learned (so far)

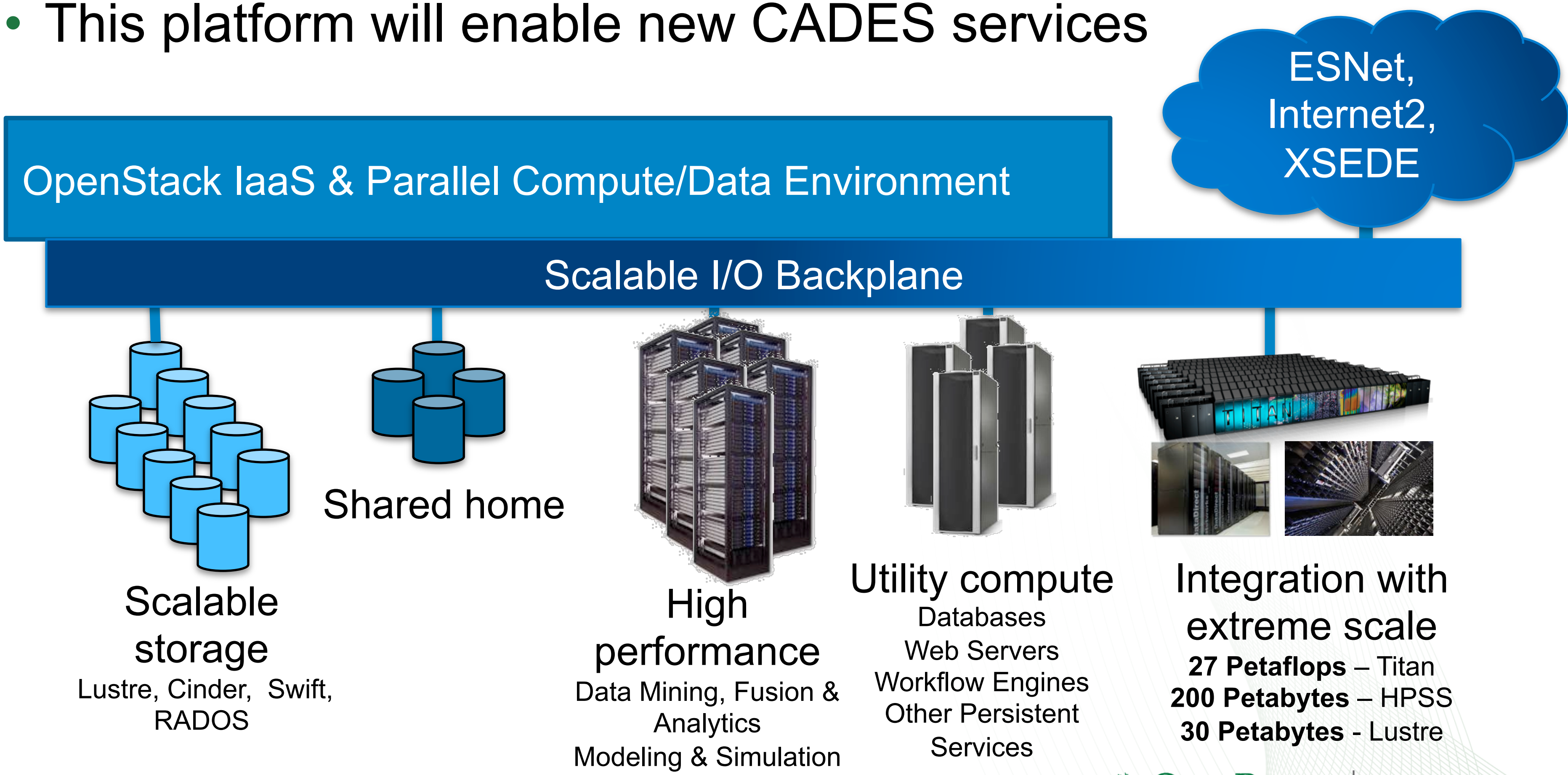
- Communication and Relationships (scientists-developers, lab-lab, component-component, etc)
- Unstructured grids and interpolation
- Messaging across heterogeneous security enclaves
- High Resolution data issues
  - Storage (HPSS)
  - Movement (Globus and security policy)

Discussion

Questions?

CADES integration with OLCF

- The CADES cloud infrastructure is a new resource that has been added to the existing services of CADES
- This platform will enable new CADES services



ESNet, Internet2, XSEDE

OpenStack IaaS & Parallel Compute/Data Environment

Scalable I/O Backplane

Scalable storage
Lustre, Cinder, Swift, RADOS

Shared home

High performance
Data Mining, Fusion & Analytics
Modeling & Simulation

Utility compute
Databases
Web Servers
Workflow Engines
Other Persistent Services

Integration with extreme scale
27 Petaflops – Titan
200 Petabytes – HPSS
30 Petabytes - Lustre

Testing and execution framework tailored for ACME

Features	Description	Impact
Infrastructure	Creates a flexible, extensible infrastructure for future ACME efforts and related DOE projects, automates laborious, repetitive simulation data tasks to improve productivity	Heightens productivity and user experience
Data Sharing	Supports broad data sharing within ACME project teams and with scientific collaborations; including NGEE, ARM, CDIAC, etc.	Accelerates model development and result dissemination
Provenance	Enables reproducibility, archiving and reuse of high-volume simulation data, provenance captures set up, execution and analysis details coupled with standard metadata creation, annotation, and forums for group discussions and sharing of any part of a workflow	Increases reproducibility, productivity and credibility of collaboration
Model set up and execution	Rule based support for model setup, specialized collaborative portal with a checklist for approvers of new model setups before job launching, Links to User interface and infrastructure for job submission	Enables new users to be effective quickly, allows control over model set ups in distributed, collaborative teams
User Interface	Specialized software when needed to enable web job submission, running, monitoring, and debugging capabilities on several HPC centers	One stop shop to all needed capabilities, increases productivity, reproducibility
Ensemble and Automated Runs	Job launching interface for submission of hundreds of production runs and enabling specialized monitoring of multiple ensemble, automated runs	Increases productivity