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ENERGY SCIENCES NETWORK

Modern Cyberinfrastructure: The Ladder to the Shoulders Of Giants

Eli Dart, Science Engagement
Energy Sciences Network (ESnet)
Lawrence Berkeley National Laboratory

PEARC20
Virtual (Coronapocalypse)
July 27, 2020

U.S. DEPARTMENT OF ENERGY
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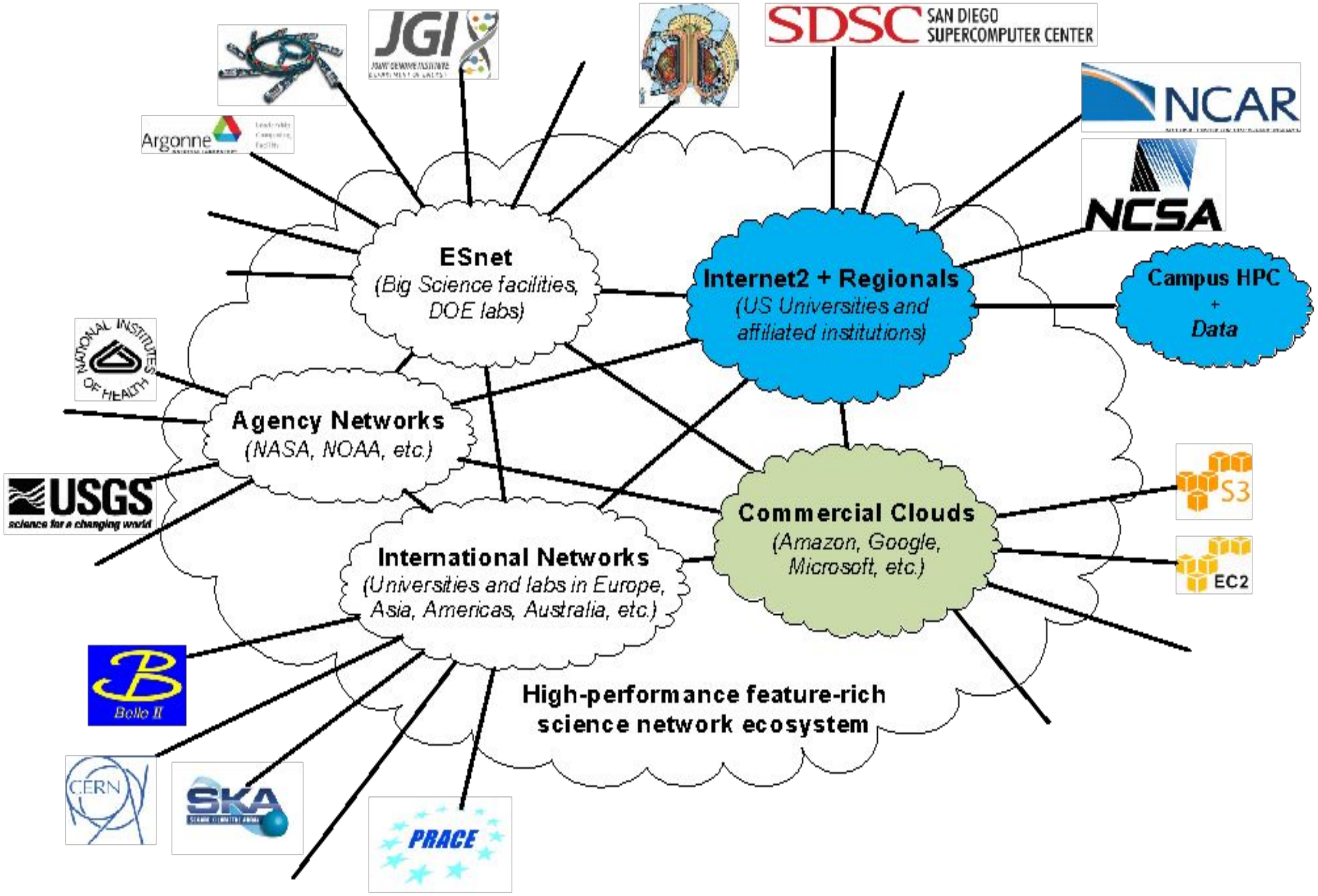
Our Community Has Made Great Progress

- Over the past 8-10 years or so, we have made great strides forward
- Science networks are big, fast, and clean
  - High speed regional and national networks
  - R&E exchanges
  - Campus networks
  - International connectivity
- Science networks are instrumented for performance
  - perfSONAR
  - Critical for ensuring correct operation
  - Invaluable for timely resolution of problems

Our Community Has Made Great Progress

- The Science DMZ model is widely deployed
  - Campuses, laboratories, experiments
  - HPC facilities
  - Some data portals (more on this later)
- DTNs in the Science DMZs
  - Connect storage to high speed networks
  - HPC filesystems
  - Experiment data acquisition systems
- Data orchestration platforms running on the DTNs
  - This is what the scientist sees
  - Capable platforms allow orchestration rather than clunky user-driven scripting or manual downloads

Data Ecosystem - Abstract Network Diagram


JGI
SDSC SAN DIEGO SUPERCOMPUTER CENTER
NCAR
NCSA
Argonne
ESnet
(Big Science facilities, DOE labs)
Internet2 + Regionals
(US Universities and affiliated institutions)
Campus HPC
+
Data
NATIONAL INSTITUTES OF HEALTH
Agency Networks
(NASA, NOAA, etc.)
USGS
science for a changing world
Commercial Clouds
(Amazon, Google, Microsoft, etc.)
S3
EC2
International Networks
(Universities and labs in Europe, Asia, Americas, Australia, etc.)
Belle II
High-performance feature-rich science network ecosystem
CERN
SKA
PRACE

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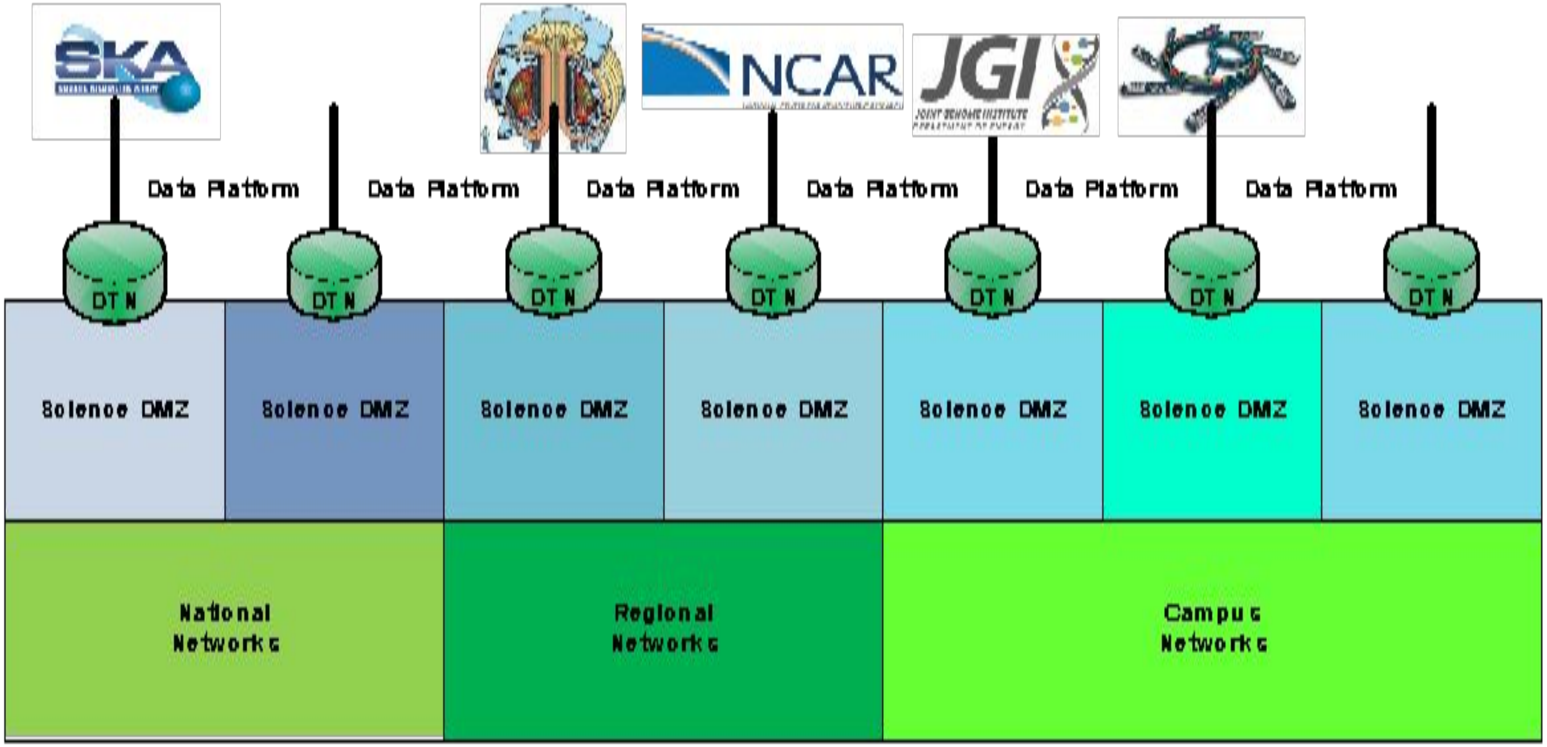
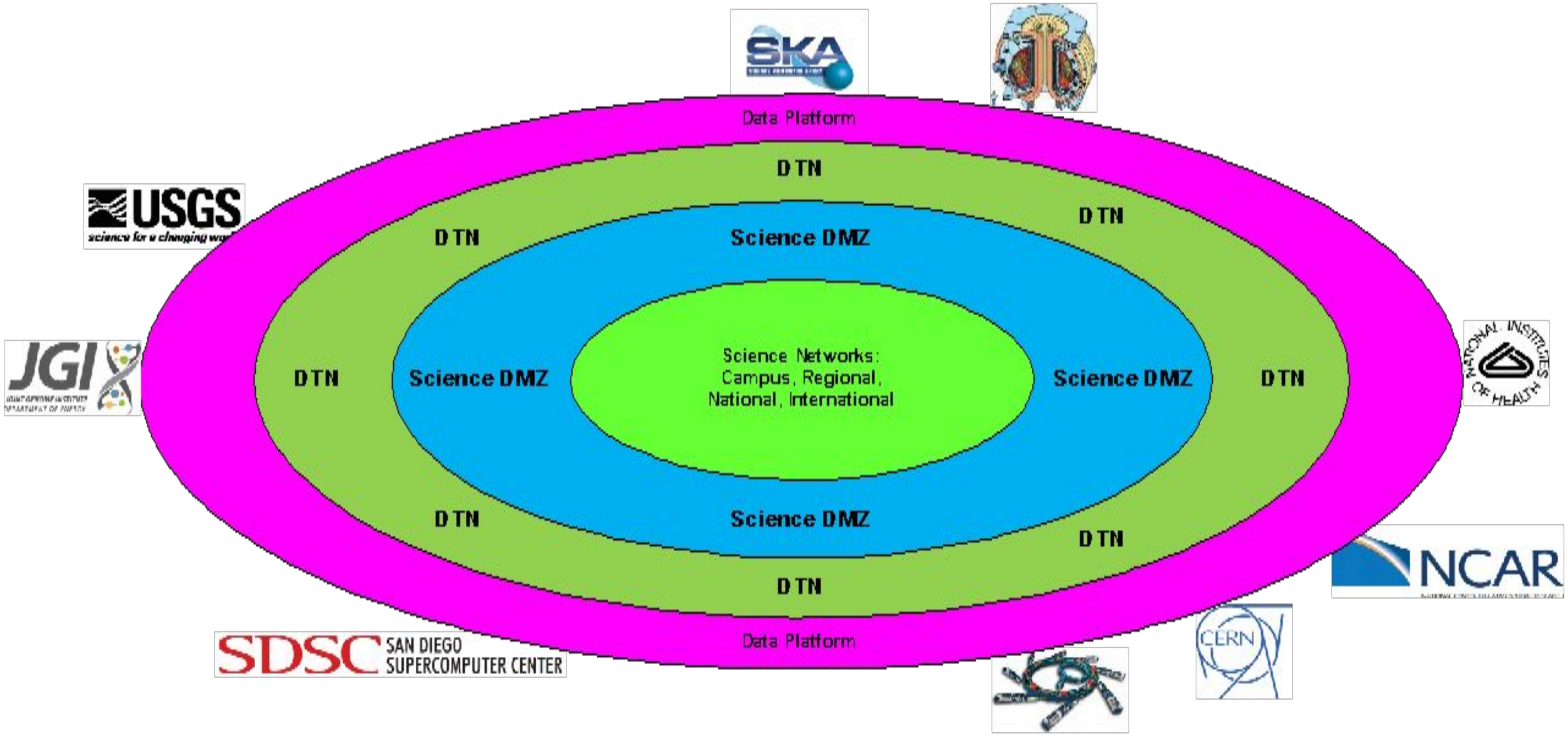
Data Ecosystem – Block Visualization



Data Ecosystem – Concentric View


Data Platform
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Science DMZ
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Science DMZ
Science Networks: Campus, Regional, National, International
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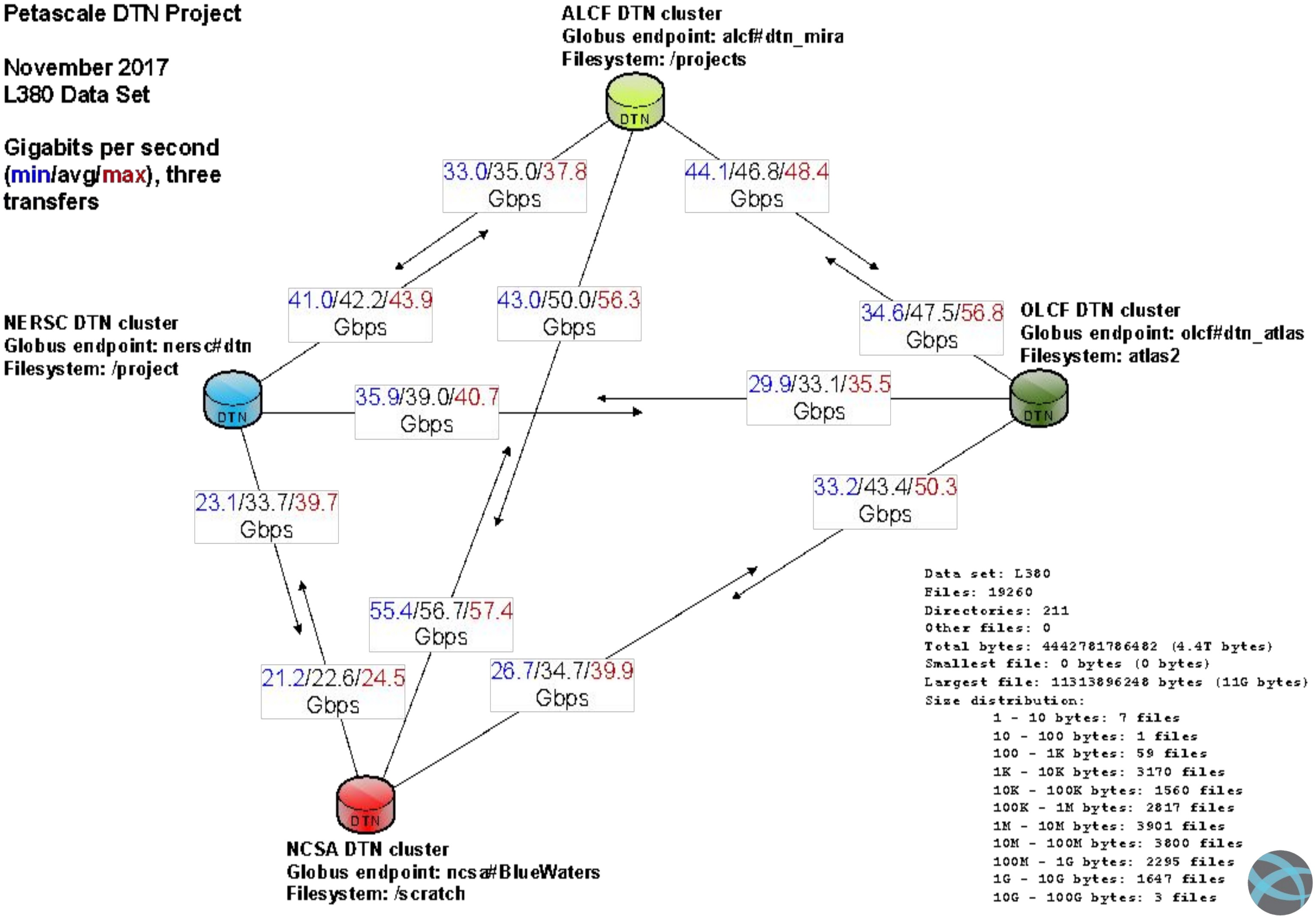
What Remains To Be Done?

- We aren’t all the way there yet (unfortunately)
- The diagrams show a vision that is not yet fully realized
- Three major tasks remain
  - Deployment of an interoperable platform across Science DMZs
    - This includes test, verification, and performance engineering
    - Partially complete
  - Integrating the major data repositories and portals with the platform
    - This has begun – lots left to do
  - Onboarding scientists and collaborations
    - Science Engagement
    - We understand it, but we need to scale it
- Remember – this has to be useful to scientists, so it has to work for them

Interoperable Platform Deployment

- This is partially complete
- Necessary features
  - Automation
  - Fault recovery
  - Data integrity
  - Integration with web-based portals
- Several platforms exist
  - Globus
    - Significant deployment in NSF and DOE spaces
    - Basis for examples shown here
  - XRootD (LHC experiments)
  - OSG Stack
- Key point – **the scientist must not be made the integrator**
  - If the scientist is the integrator, they will use HTTP and rsync+SSH forever
  - The old tools don't scale, but the scientists can't build the better platforms themselves
  - **WE** MUST DO THIS

Example Of Platform Power (Petascale DTN)



Petascale DTN Project

November 2017
L380 Data Set

Gigabits per second (min/avg/max), three transfers

```
Data set: L380
Files: 19260
Directories: 211
Other files: 0
Total bytes: 4442781786482 (4.4T bytes)
Smallest file: 0 bytes (0 bytes)
Largest file: 11313896248 bytes (11G bytes)
Size distribution:
        1 - 10 bytes: 7 files
        10 - 100 bytes: 1 files
        100 - 1K bytes: 59 files
        1K - 10K bytes: 3170 files
        10K - 100K bytes: 1560 files
        100K - 1M bytes: 2817 files
        1M - 10M bytes: 3901 files
        10M - 100M bytes: 3800 files
        100M - 1G bytes: 2295 files
        1G - 10G bytes: 1647 files
        10G - 100G bytes: 3 files
```

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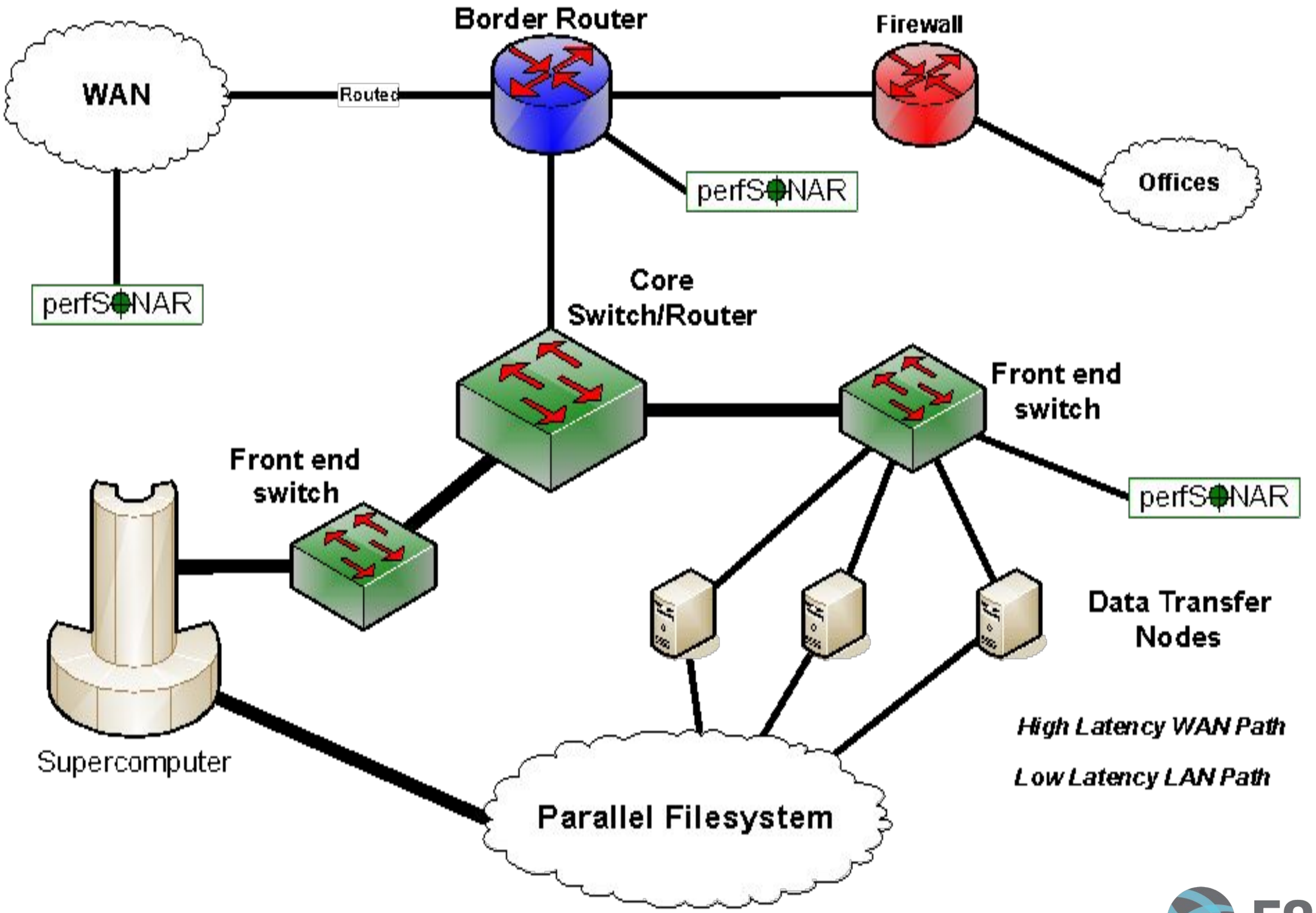
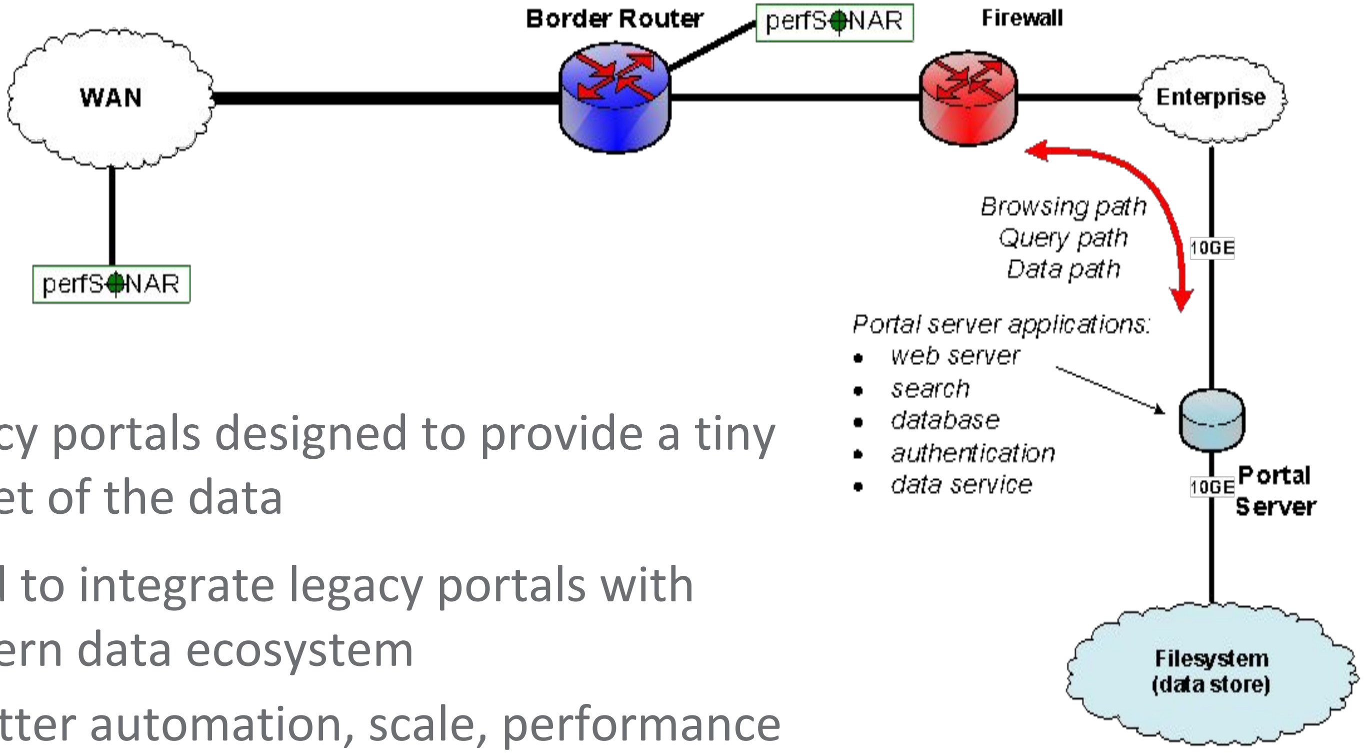
Science DMZ – HPC Center DTN Cluster



Science Data Portals

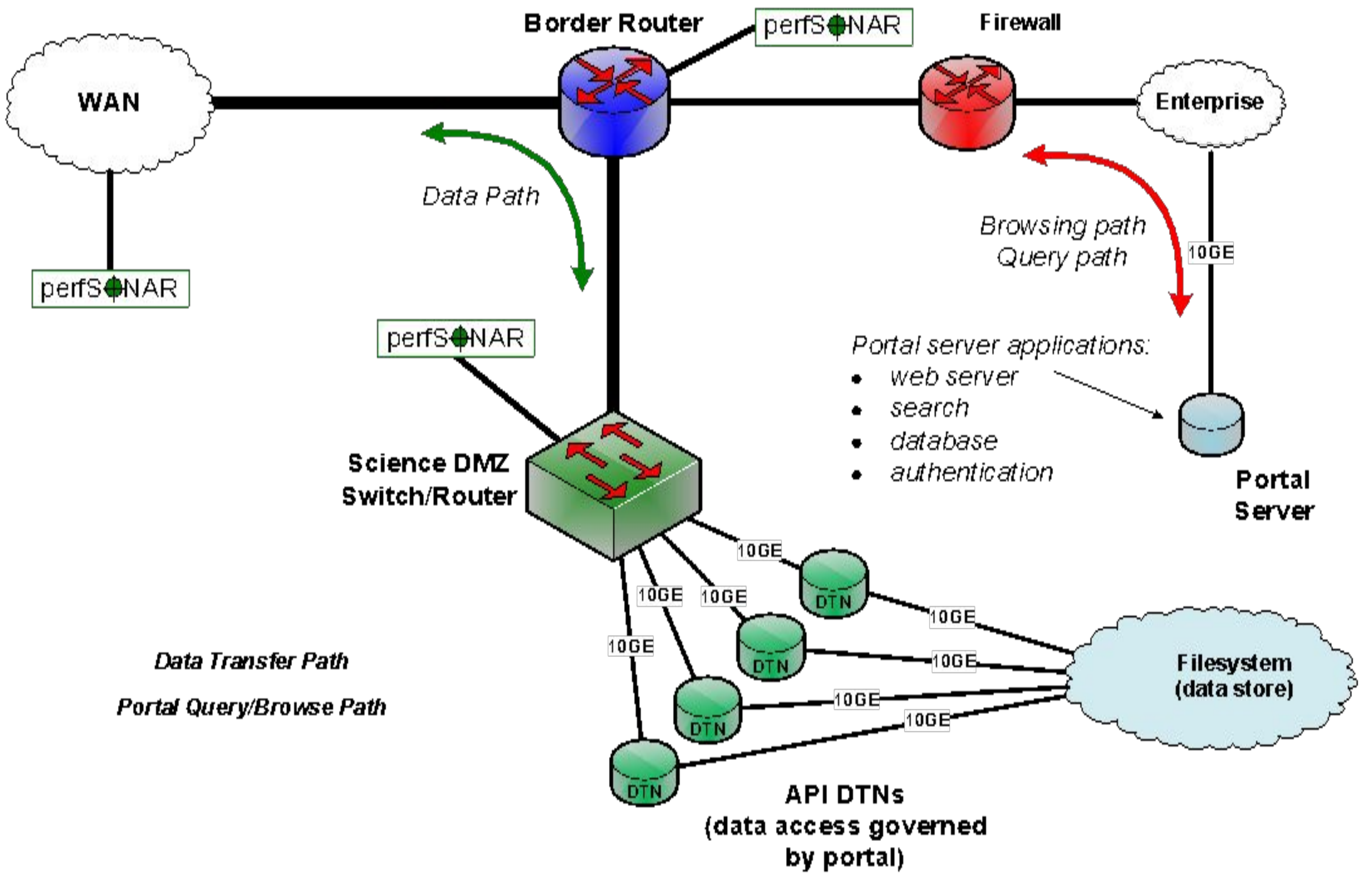
- Large repositories of scientific data
  - Climate data
  - Sky surveys (astronomy, cosmology)
  - Many others
  - Data search, browsing, access
- Many scientific data portals were designed 15+ years ago
  - Single-web-server design
  - Data browse/search, data access, user awareness all in a single system
  - All the data goes through the portal server
    - In many cases by design
    - E.g. embargo before publication (enforce access control)
  - Better than old command-line FTP, but outdated by today’s standards

Legacy Portal Design



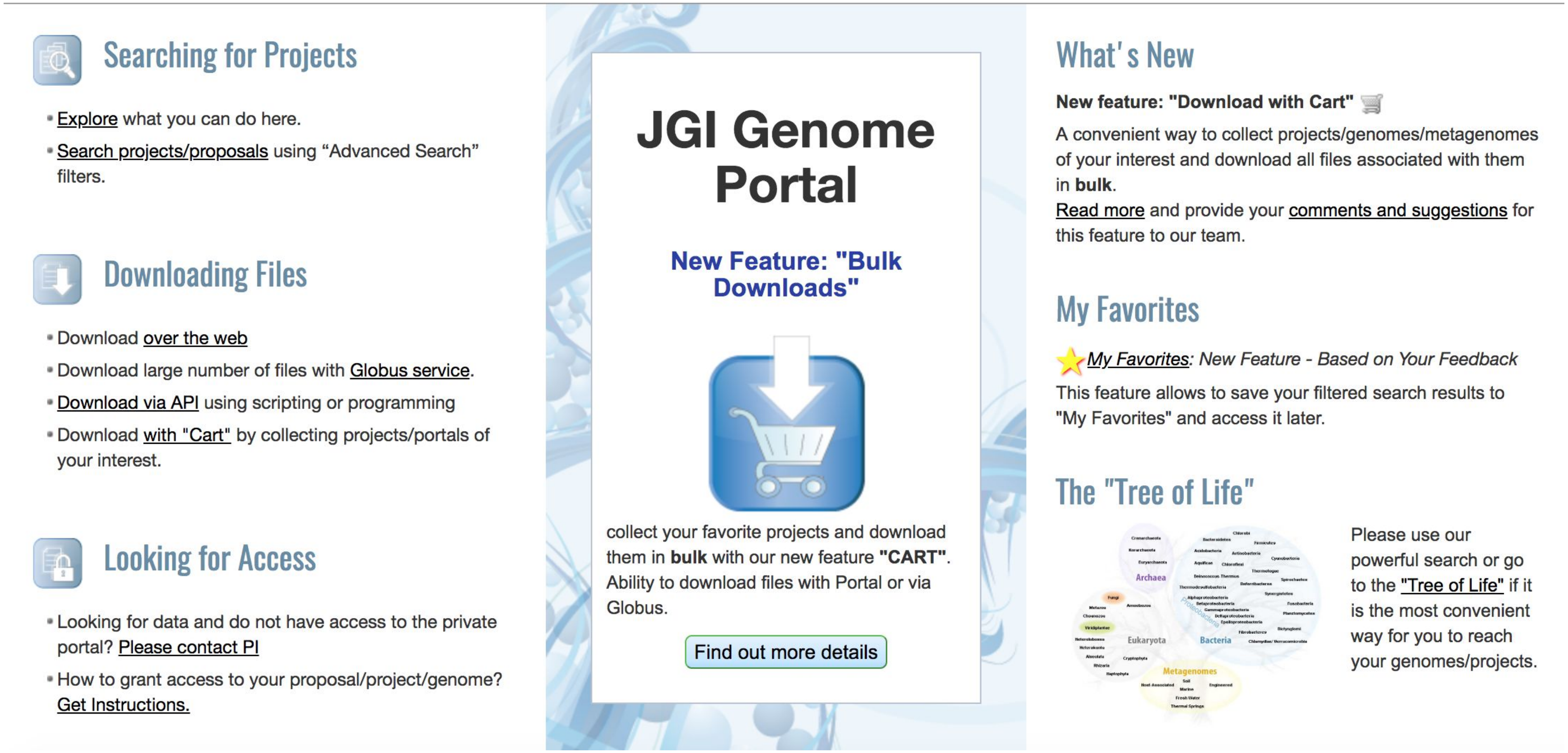
- Legacy portals designed to provide a tiny subset of the data
- Need to integrate legacy portals with modern data ecosystem
  - Better automation, scale, performance
  - Connectivity to HPC

Next-Generation Portal Leverages Science DMZ



https://peerj.com/articles/cs-144/

JGI Data Portal



Searching for Projects

- Explore what you can do here.
- Search projects/proposals using "Advanced Search" filters.

Downloading Files

- Download over the web
- Download large number of files with Globus service.
- Download via API using scripting or programming
- Download with "Cart" by collecting projects/portals of your interest.

Looking for Access

- Looking for data and do not have access to the private portal? Please contact PI
- How to grant access to your proposal/project/genome? Get Instructions.

JGI Genome Portal

New Feature: "Bulk Downloads"

collect your favorite projects and download them in **bulk** with our new feature **"CART"**. Ability to download files with Portal or via Globus.

Find out more details

What's New

New feature: "Download with Cart"

A convenient way to collect projects/genomes/metagenomes of your interest and download all files associated with them in **bulk**.
Read more and provide your comments and suggestions for this feature to our team.

My Favorites

★*My Favorites: New Feature - Based on Your Feedback*

This feature allows to save your filtered search results to "My Favorites" and access it later.

The "Tree of Life"

Please use our powerful search or go to the "Tree of Life" if it is the most convenient way for you to reach your genomes/projects.

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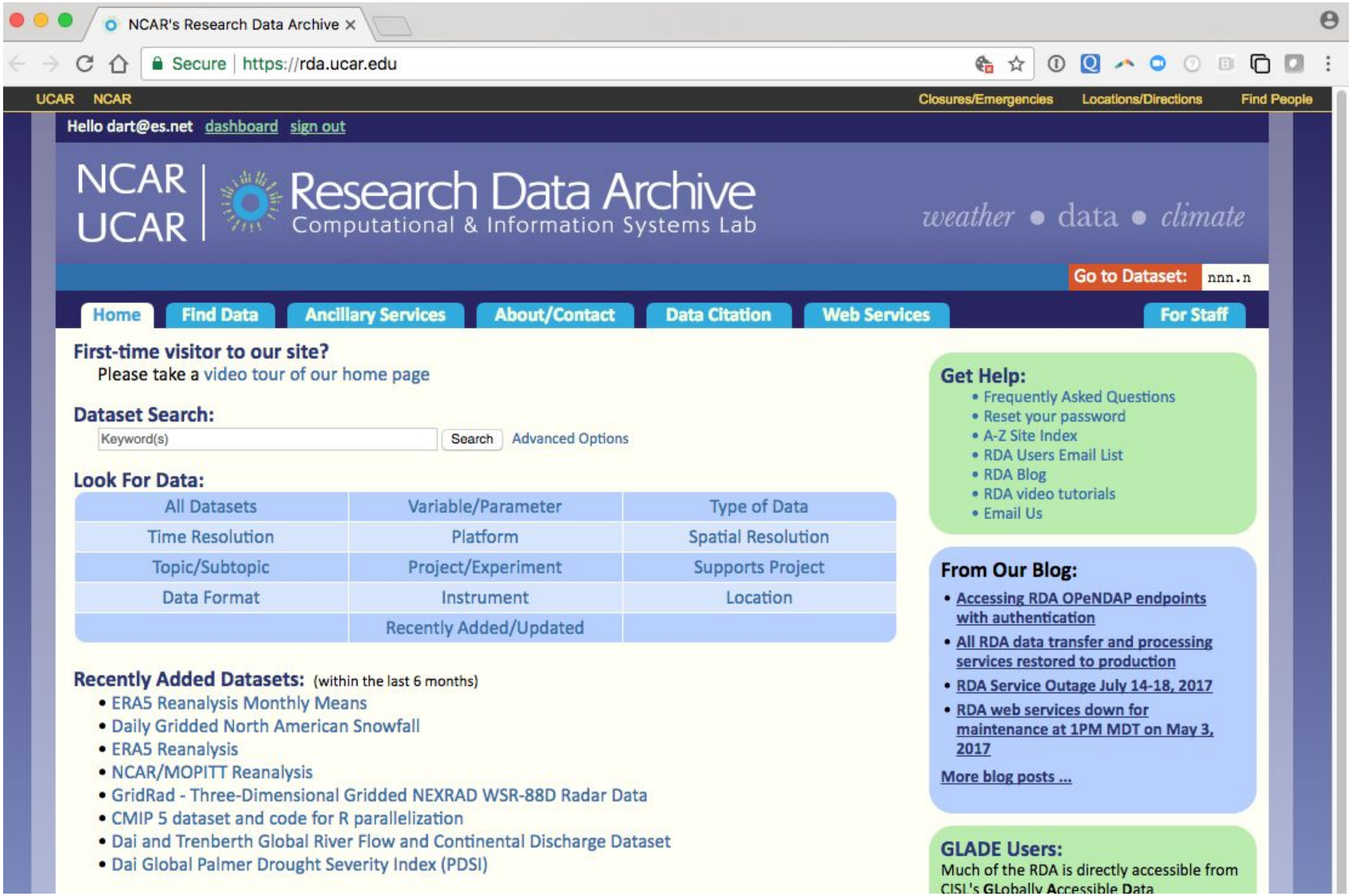

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NCAR UCAR
Research Data Archive
Computational & Information Systems Lab
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- CMIP 5 dataset and code for R parallelization
- Dai and Trenberth Global River Flow and Continental Discharge Dataset
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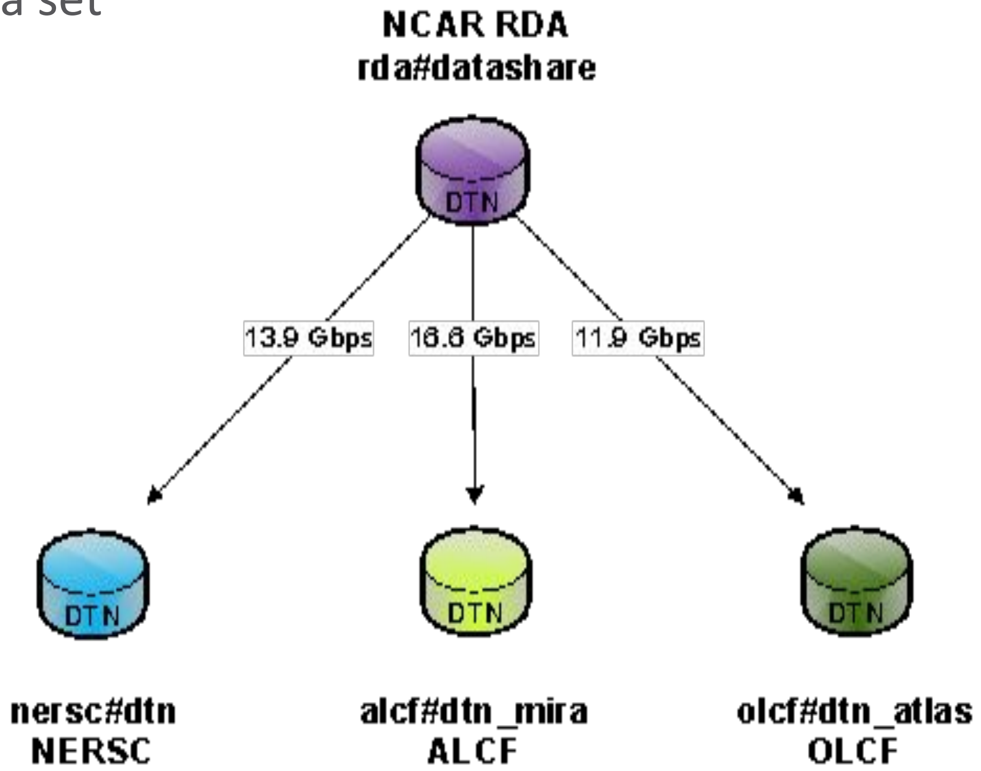
More blog posts ...

GLADE Users:
Much of the RDA is directly accessible from CISL's GLobally Accessible Data

NCAR RDA Performance to DOE HPC Facilities

- 1.5TB data set
- 1121 files



NCAR RDA
rda#datashare

DTN

13.9 Gbps

16.8 Gbps

11.9 Gbps

DTN

nersc#dtn
NERSC

DTN

alcf#dtn_mira
ALCF

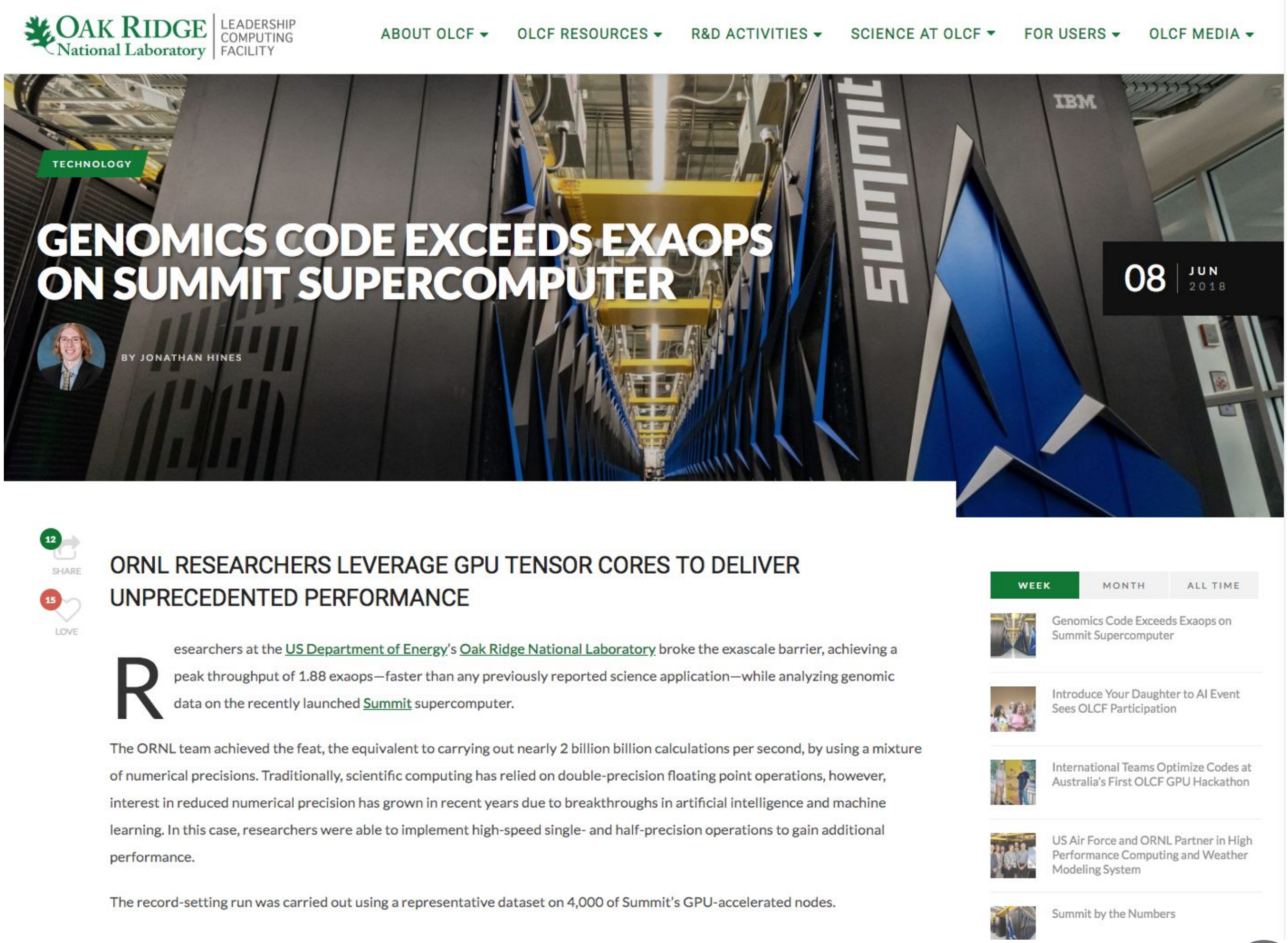
DTN

olcf#dtn_atlas
OLCF

Reasons To Scale Data Portals

- Some reasons are obvious
  - Increase in size of data objects (MB □ GB □ 100s of GB)
  - Number of data objects (many thousands per data set)
- Other reasons are paradigm shifts
  - Modern data analysis on HPC can use a *lot* of data
  - Today’s HPC facilities are far more capable than in the past
- Retrofit / rebuilt data portals and data repositories
  - Significant wins from increased data analysis

Science at Scale: Genomics



GENOMICS CODE EXCEEDS EXAOPS ON SUMMIT SUPERCOMPUTER

BY JONATHAN HINES

08 JUN 2018

ORNL RESEARCHERS LEVERAGE GPU TENSOR CORES TO DELIVER UNPRECEDENTED PERFORMANCE

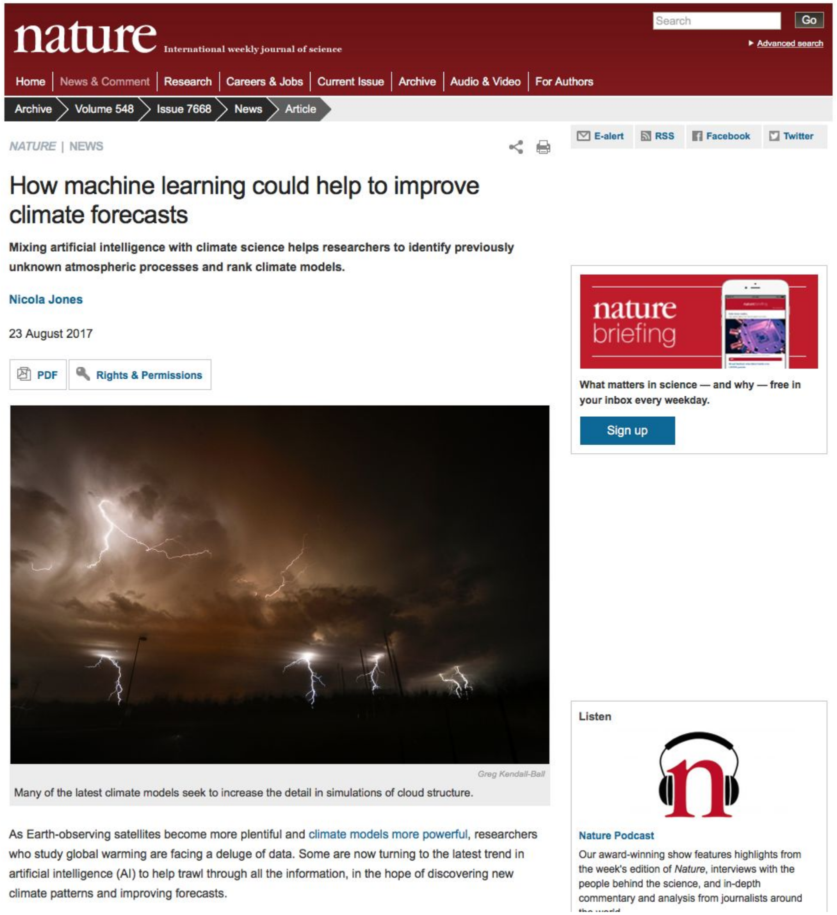
Researchers at the US Department of Energy's Oak Ridge National Laboratory broke the exascale barrier, achieving a peak throughput of 1.88 exaops—faster than any previously reported science application—while analyzing genomic data on the recently launched Summit supercomputer.

The ORNL team achieved the feat, the equivalent to carrying out nearly 2 billion billion calculations per second, by using a mixture of numerical precisions. Traditionally, scientific computing has relied on double-precision floating point operations, however, interest in reduced numerical precision has grown in recent years due to breakthroughs in artificial intelligence and machine learning. In this case, researchers were able to implement high-speed single- and half-precision operations to gain additional performance.

The record-setting run was carried out using a representative dataset on 4,000 of Summit's GPU-accelerated nodes.

- Genomics Code Exceeds Exaops on Summit Supercomputer
- Introduce Your Daughter to AI Event Sees OLCF Participation
- International Teams Optimize Codes at Australia's First OLCF GPU Hackathon
- US Air Force and ORNL Partner in High Performance Computing and Weather Modeling System
- Summit by the Numbers

Science at Scale: Climate



NATURE | NEWS

How machine learning could help to improve climate forecasts

Mixing artificial intelligence with climate science helps researchers to identify previously unknown atmospheric processes and rank climate models.

Nicola Jones

23 August 2017

Greg Kendall-Ball

Many of the latest climate models seek to increase the detail in simulations of cloud structure.

As Earth-observing satellites become more plentiful and climate models more powerful, researchers who study global warming are facing a deluge of data. Some are now turning to the latest trend in artificial intelligence (AI) to help trawl through all the information, in the hope of discovering new climate patterns and improving forecasts.

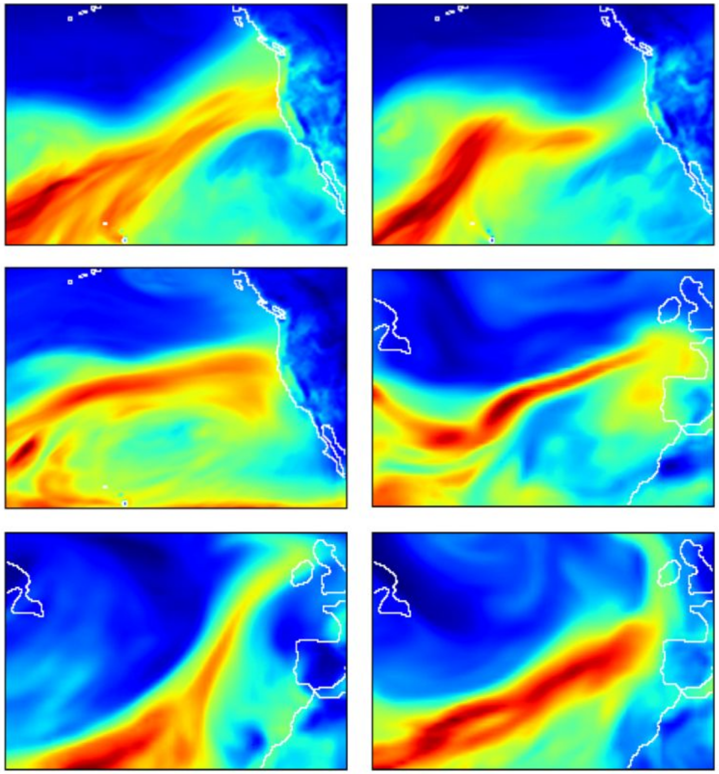


Figure 3: Sample images of atmospheric rivers correctly classified (true positive) by our deep CNN model. Figure shows total column water vapor (color map) and land sea boundary (solid line).

They Can Use All The Data

- Groups like these need large data sets
- Much of the data in their field is behind legacy portals
  - Significant human effort to retrieve what they need
  - Legacy systems perform poorly, especially at scale
- Legacy data portals are a product of their time
  - Remember: these were designed to serve small data to small systems
  - We now live in the future from the perspective of those designs
  - Current systems far exceed the capabilities available 15 years ago
  - From the perspective of today’s systems, legacy portals are products of a bygone past
- It is now perfectly reasonable for a scientist to want all the data
  - Machine learning + HPC
  - But this only works if the scientists can get to the data at scale

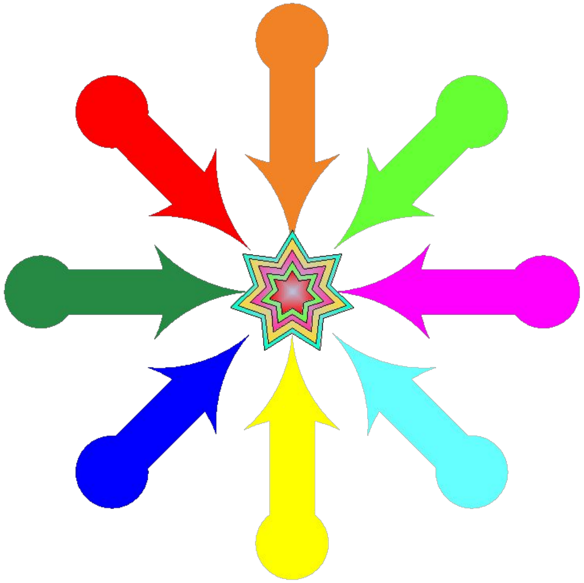
We (not the scientists) Have To Do This

- The scientific community cannot do this for themselves
- Individual researchers do not control the resources
  - Computing centers
  - Data repositories
  - Science networks
  - Our community owns these – we have to do the work
- Integration, performance engineering, interoperability
- Science Engagement to teach scientists how to use the better platforms
- This is the path forward

¯_(ツ)_/¯

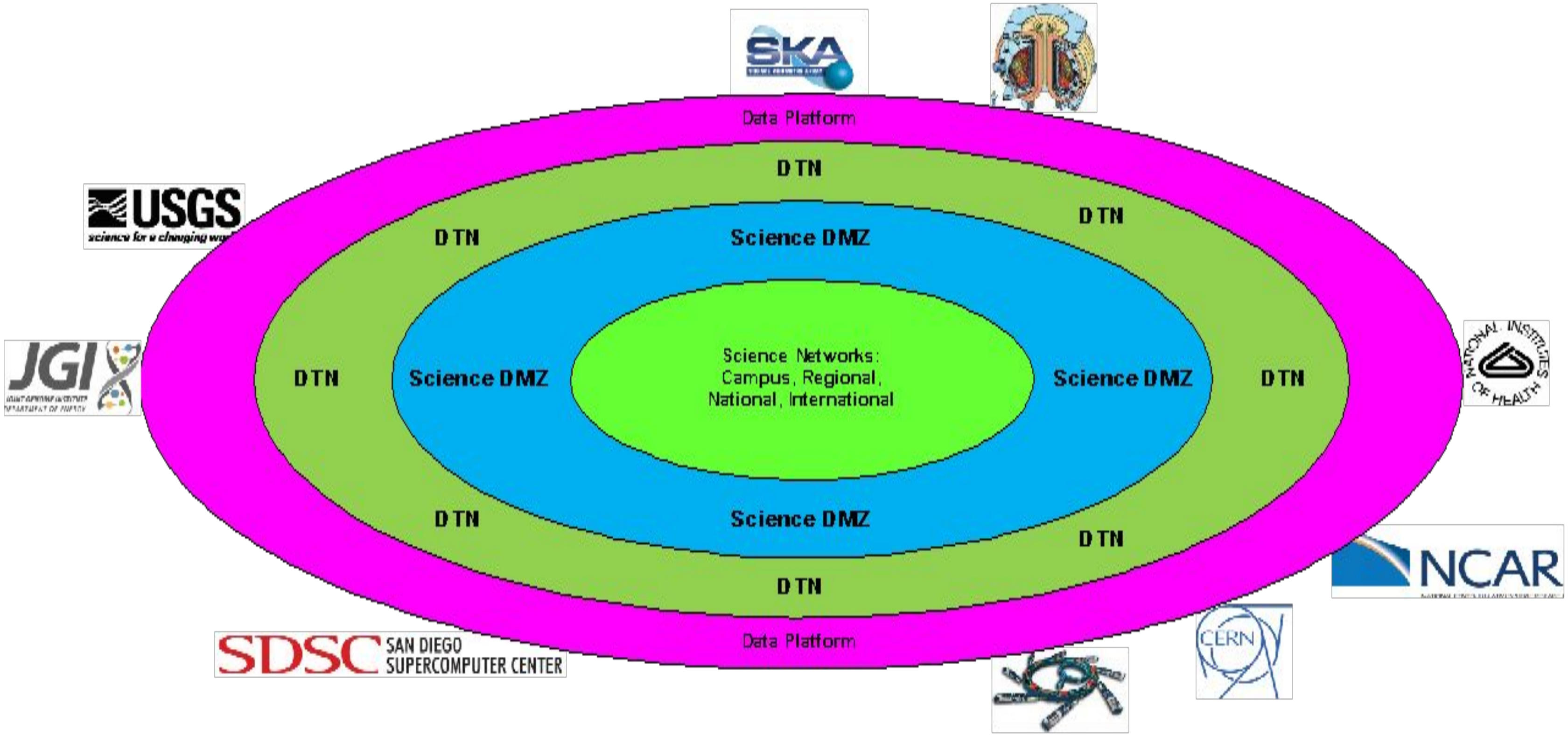
Networks Cannot Do This Alone

- We need a whole-community effort
  - Networks
  - HPC facilities
  - Data repositories / Data portals
  - Experimental facilities
  - Science collaborations
  - Science programs



- Networks can help, and must be part of the conversation
  - Heavy lifting is now at the network edge, in collaboration with the network core
  - Need to help them get the architecture right – we know how to do this

Vision – Interoperable Computing And Data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Science DMZ
DTN
DTN
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CERN

Cyberinfrastructure Is The Ladder Up

- An integrated, interoperable cyberinfrastructure will allow scientists to make effective use of data, computing, and networks
- This is how we will achieve the advances we need in medicine, energy, climate science, and many other fields
- Large-scale data can only be effectively used if the tools work well together - otherwise the effort is too great

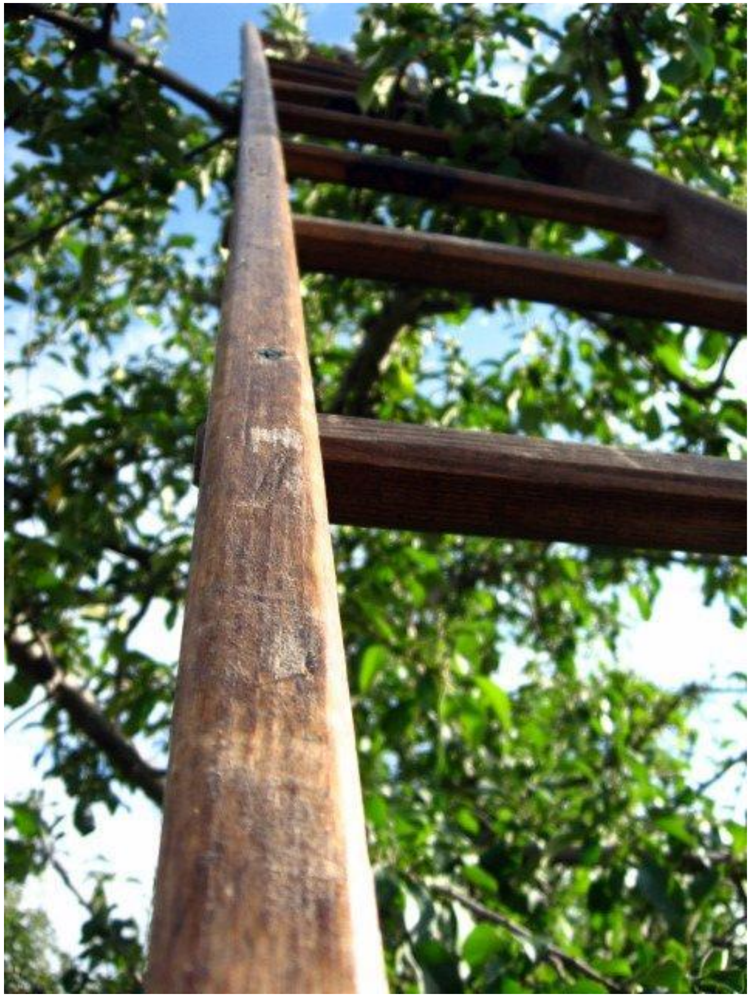

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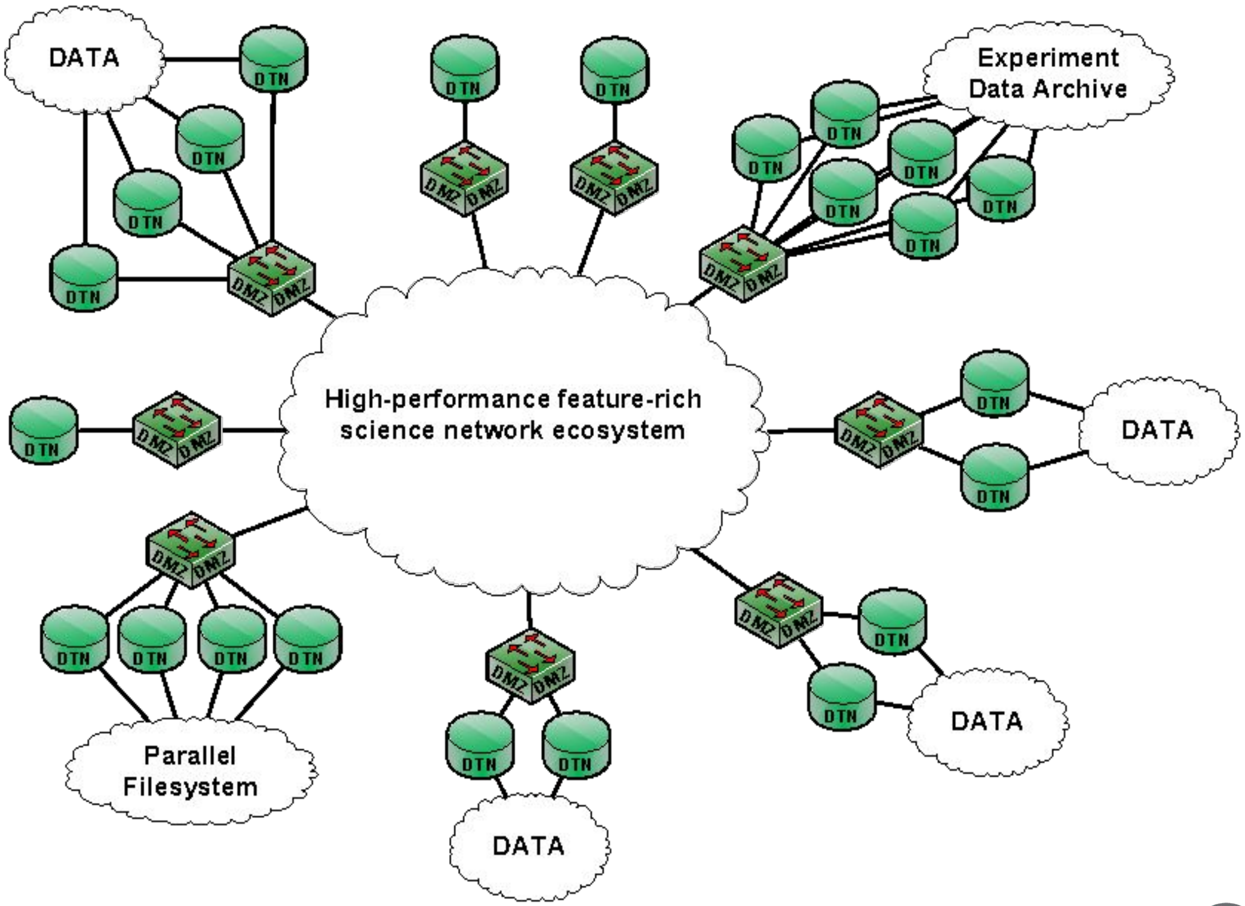
Image credit: https://www.flickr.com/photos/amylovesyah/ (CC BY 2.0)

The Path Forward



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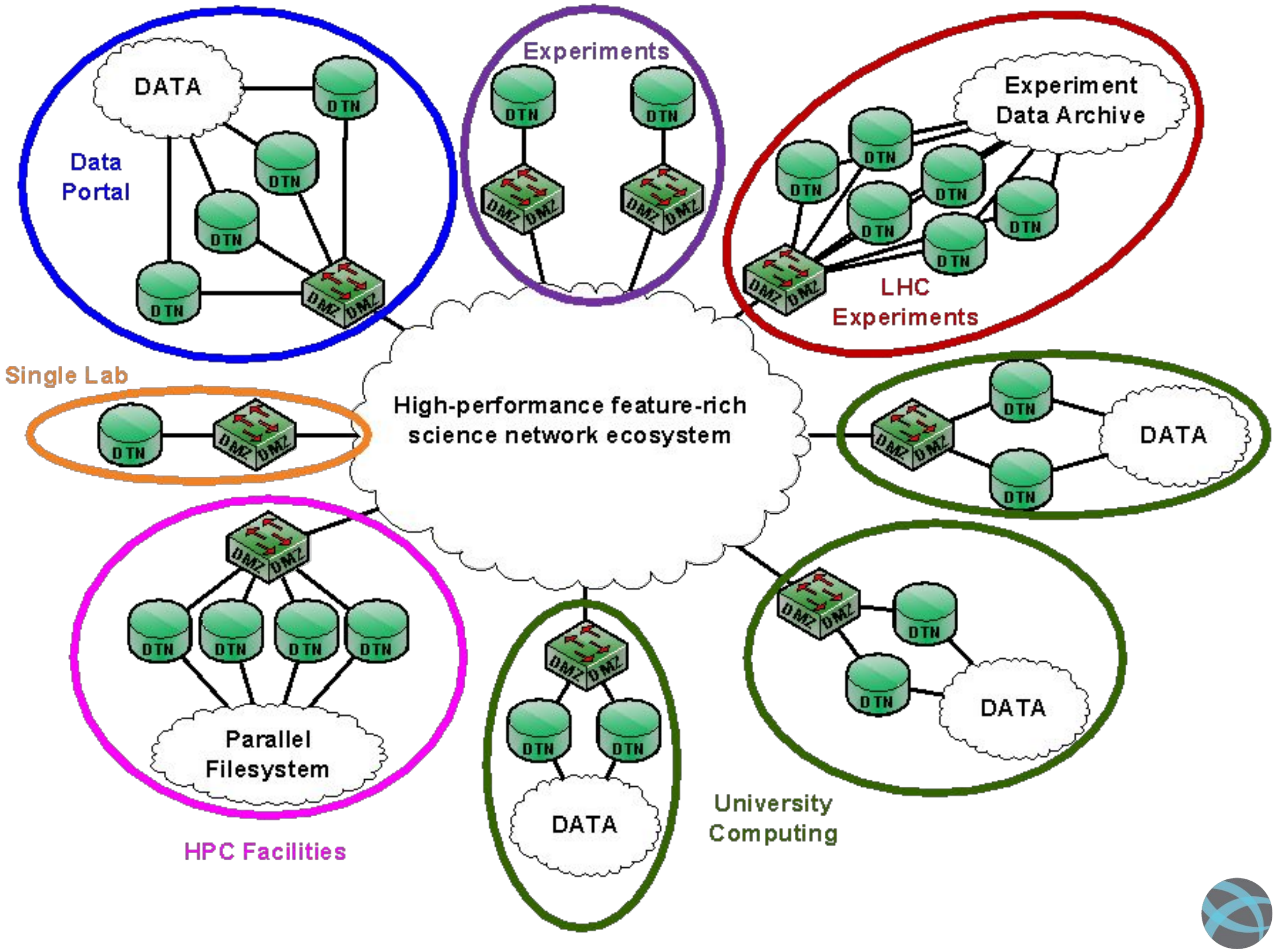

Standing On The Shoulders Of Giants

- Large-scale data sets are the giants of today
- We have all the components we need to give all scientists access to all the data in their fields
- This is not a design problem
  - We have the designs, the technologies, the models
  - We know it works: we have examples
- This is an integration and deployment problem
  - We know what we need to do
  - Let's get to it!

Isaac Newton

Image source: https://commons.wikimedia.org/wiki/File:Sir_Isaac_Newton_by_Sir_Godfrey_Kneller,_Bt.jpg
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Thanks!

Eli Dart dart@es.net

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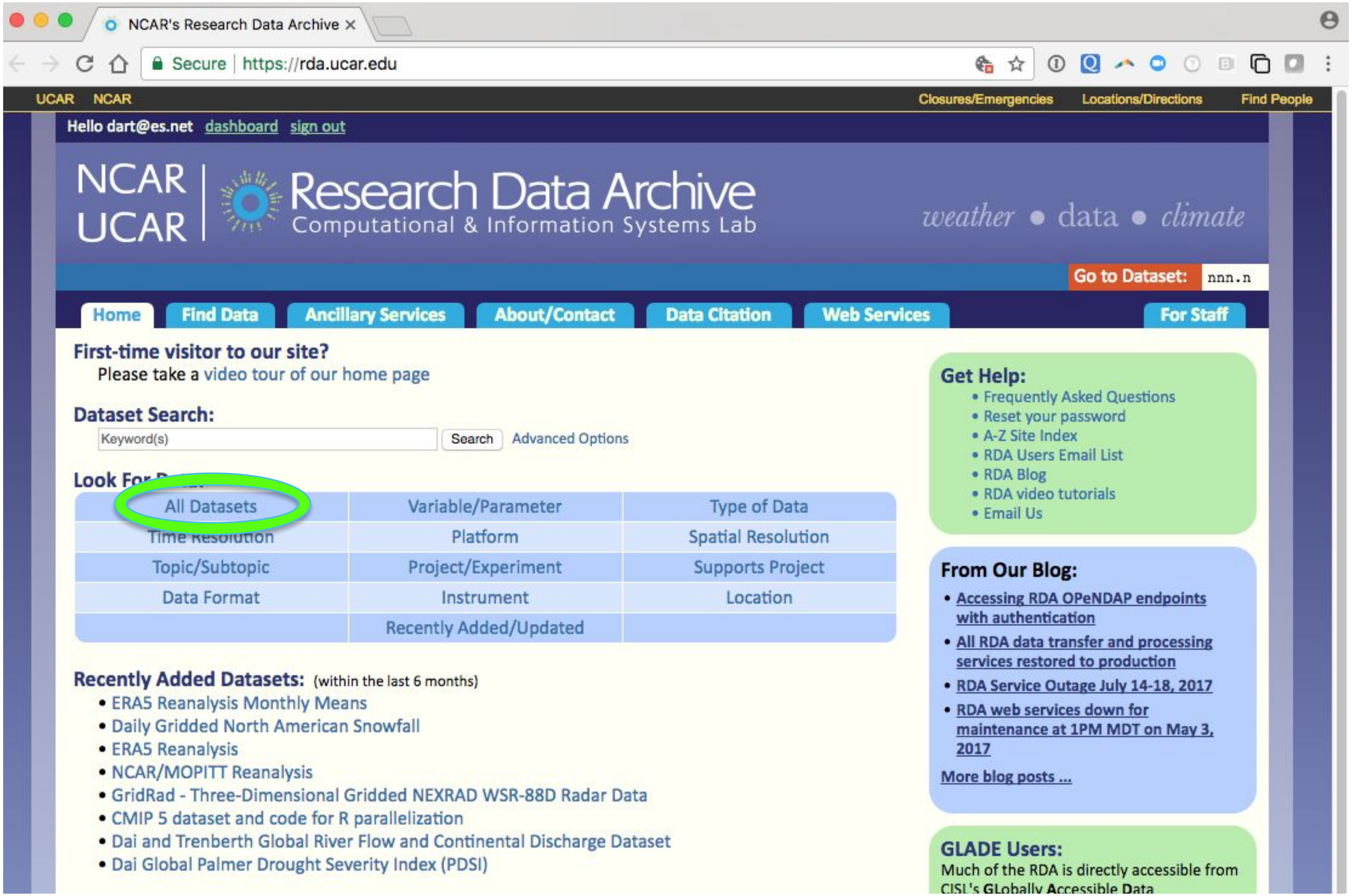
Extra slides – data download from portal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Time Resolution	Platform	Spatial Resolution
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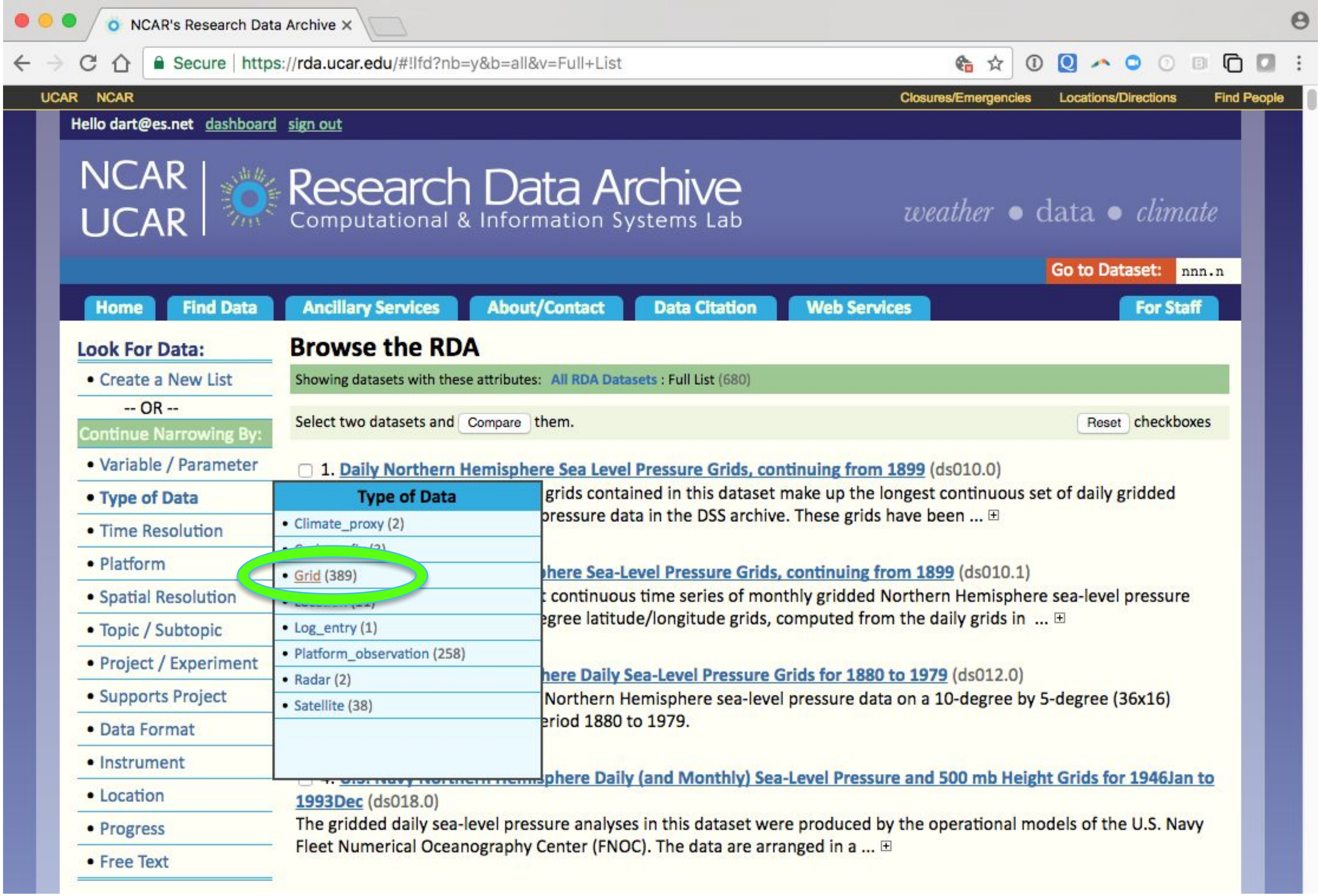
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-- OR --

Continue Narrowing By:

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- Platform
- Spatial Resolution
- Topic / Subtopic
- Project / Experiment
- Supports Project
- Data Format
- Instrument
- Location
- Progress
- Free Text

Showing datasets with these attributes: All RDA Datasets : Full List (680)

Select two datasets and Compare them. Reset checkboxes

Type of Data

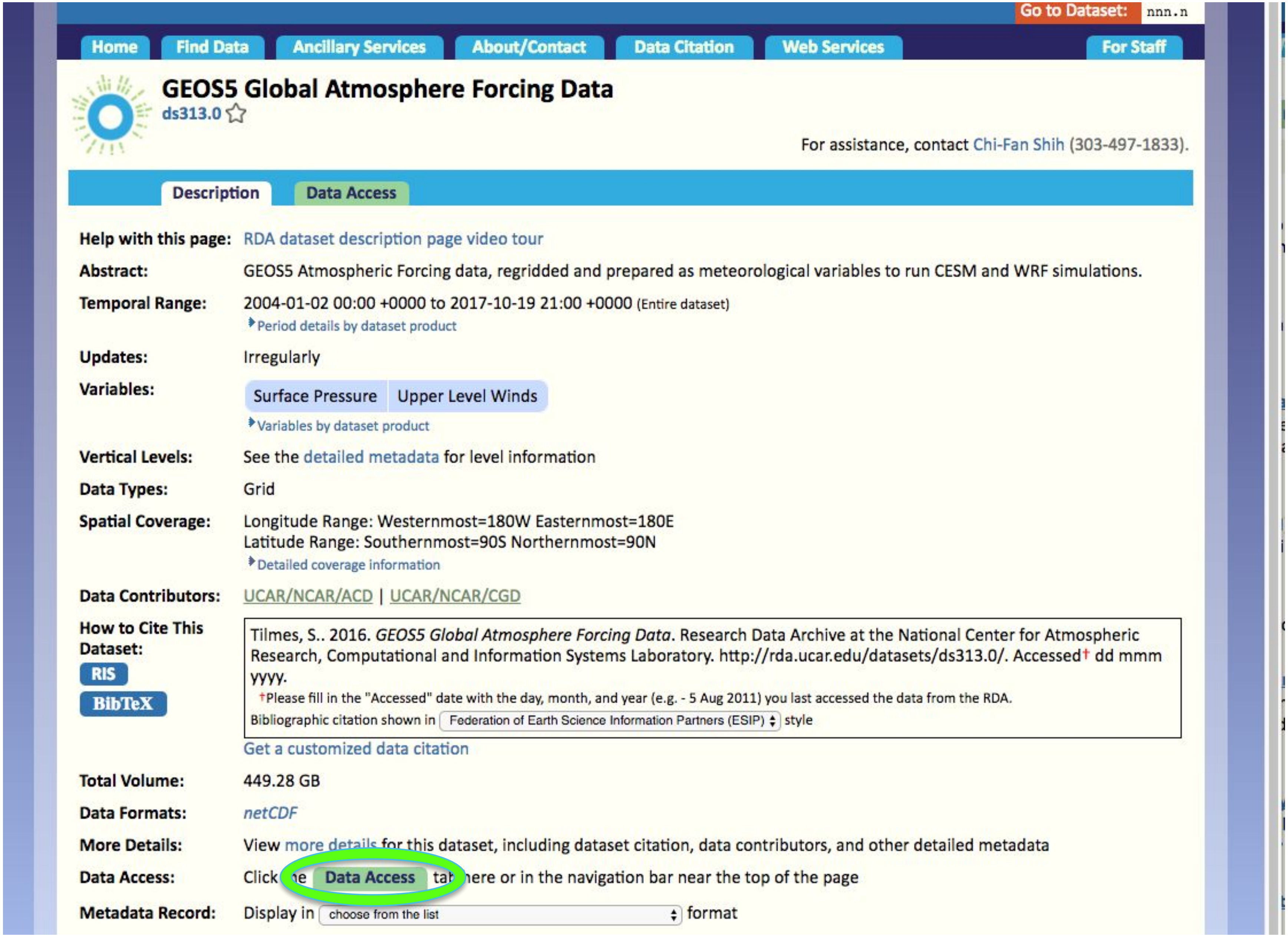
- Climate_proxy (2)
- Grid (389)
- Log_entry (1)
- Platform_observation (258)
- Radar (2)
- Satellite (38)

□ 1. Daily Northern Hemisphere Sea Level Pressure Grids, continuing from 1899 (ds010.0)
grids contained in this dataset make up the longest continuous set of daily gridded pressure data in the DSS archive. These grids have been ... ⊞

here Sea-Level Pressure Grids, continuing from 1899 (ds010.1)
continuous time series of monthly gridded Northern Hemisphere sea-level pressure egree latitude/longitude grids, computed from the daily grids in ... ⊞

here Daily Sea-Level Pressure Grids for 1880 to 1979 (ds012.0)
Northern Hemisphere sea-level pressure data on a 10-degree by 5-degree (36x16) eriod 1880 to 1979.

phere Daily (and Monthly) Sea-Level Pressure and 500 mb Height Grids for 1946Jan to 1993Dec (ds018.0)
The gridded daily sea-level pressure analyses in this dataset were produced by the operational models of the U.S. Navy Fleet Numerical Oceanography Center (FNOC). The data are arranged in a ... ⊞



GEOS5 Global Atmosphere Forcing Data

ds313.0 ☆

For assistance, contact Chi-Fan Shih (303-497-1833).

Help with this page: RDA dataset description page video tour

Abstract: GEOS5 Atmospheric Forcing data, regridded and prepared as meteorological variables to run CESM and WRF simulations.

Temporal Range: 2004-01-02 00:00 +0000 to 2017-10-19 21:00 +0000 (Entire dataset)
Period details by dataset product

Updates: Irregularly

Variables: Surface Pressure | Upper Level Winds
Variables by dataset product

Vertical Levels: See the detailed metadata for level information

Data Types: Grid

Spatial Coverage: Longitude Range: Westernmost=180W Easternmost=180E
Latitude Range: Southernmost=90S Northernmost=90N
Detailed coverage information

Data Contributors: UCAR/NCAR/ACD | UCAR/NCAR/CGD

How to Cite This Dataset: RIS BibTeX

Tilmes, S.. 2016. *GEOS5 Global Atmosphere Forcing Data*. Research Data Archive at the National Center for Atmospheric Research, Computational and Information Systems Laboratory. http://rda.ucar.edu/datasets/ds313.0/. Accessed† dd mmm yyyy.

†Please fill in the "Accessed" date with the day, month, and year (e.g. - 5 Aug 2011) you last accessed the data from the RDA.

Bibliographic citation shown in Federation of Earth Science Information Partners (ESIP) style

Get a customized data citation

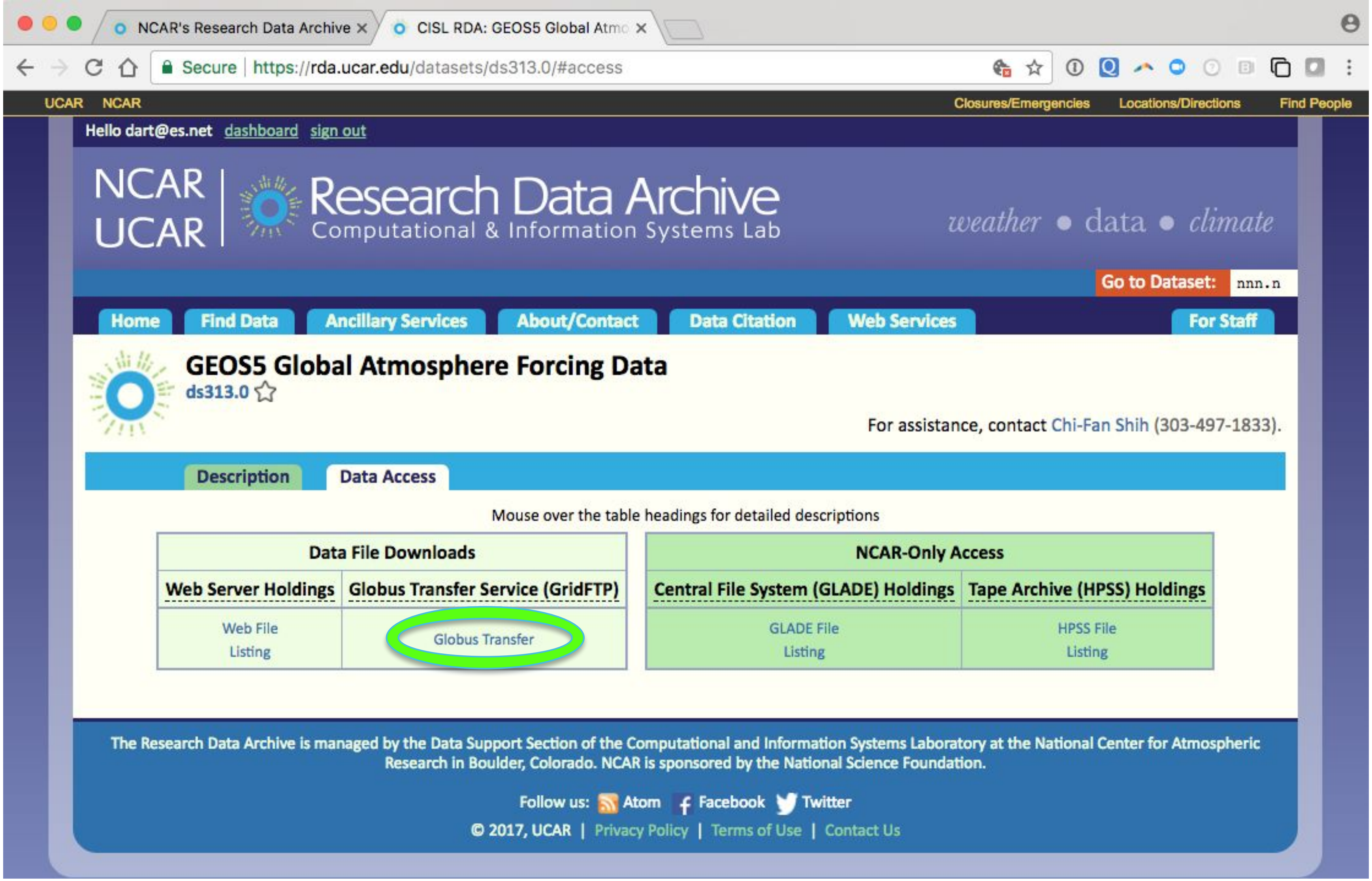
Total Volume: 449.28 GB

Data Formats: *netCDF*

More Details: View more details for this dataset, including dataset citation, data contributors, and other detailed metadata

Data Access: Click the Data Access tab here or in the navigation bar near the top of the page

Metadata Record: Display in choose from the list format



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Secure | https://rda.ucar.edu/datasets/ds313.0/#access

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GEOS5 Global Atmosphere Forcing Data

ds313.0

For assistance, contact Chi-Fan Shih (303-497-1833).

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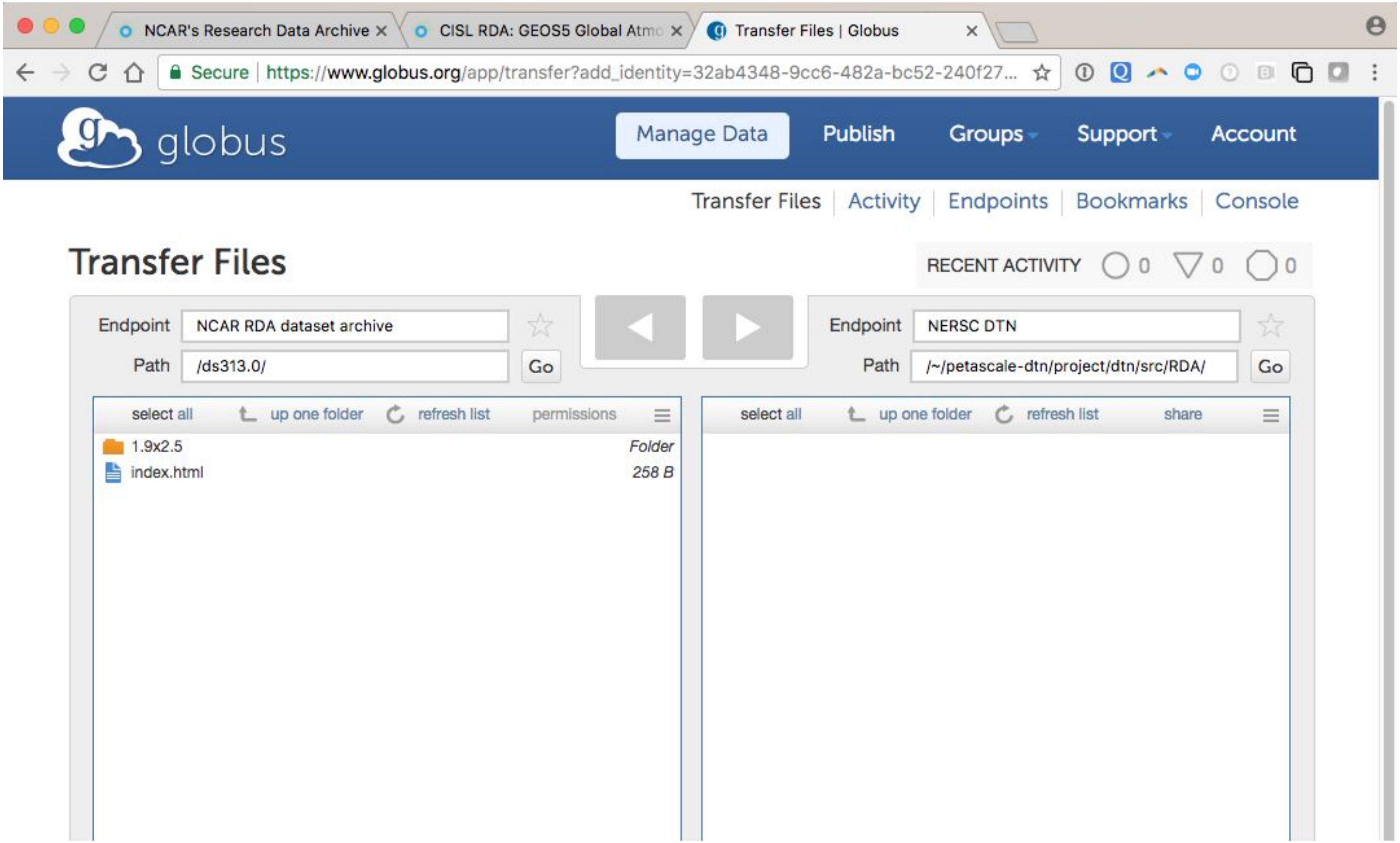
Data File Downloads		NCAR-Only Access	
Web Server Holdings	Globus Transfer Service (GridFTP)	Central File System (GLADE) Holdings	Tape Archive (HPSS) Holdings
Web File Listing	Globus Transfer	GLADE File Listing	HPSS File Listing

The Research Data Archive is managed by the Data Support Section of the Computational and Information Systems Laboratory at the National Center for Atmospheric Research in Boulder, Colorado. NCAR is sponsored by the National Science Foundation.

Portal creates a Globus transfer job for us



https://www.globus.org/app/transfer?add_identity=32ab4348-9cc6-482a-bc52-240f27...

Transfer Files

Endpoint: NCAR RDA dataset archive

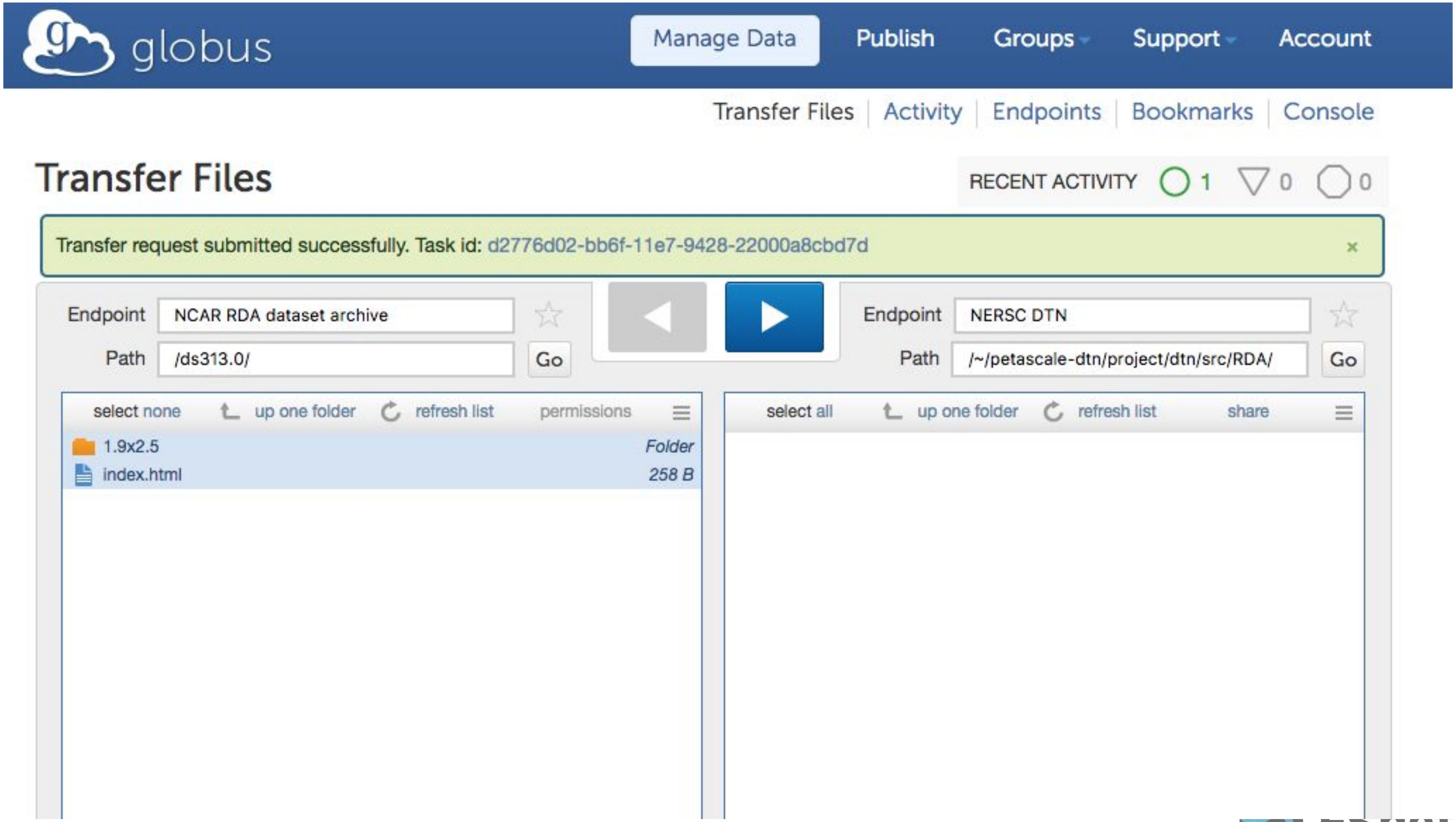
Path: /ds313.0/

1.9x2.5	*Folder*
index.html	*258 B*

Endpoint: NERSC DTN

Path: /~/petascale-dtn/project/dtn/src/RDA/

Submit the transfer job, go about our business



Transfer Files

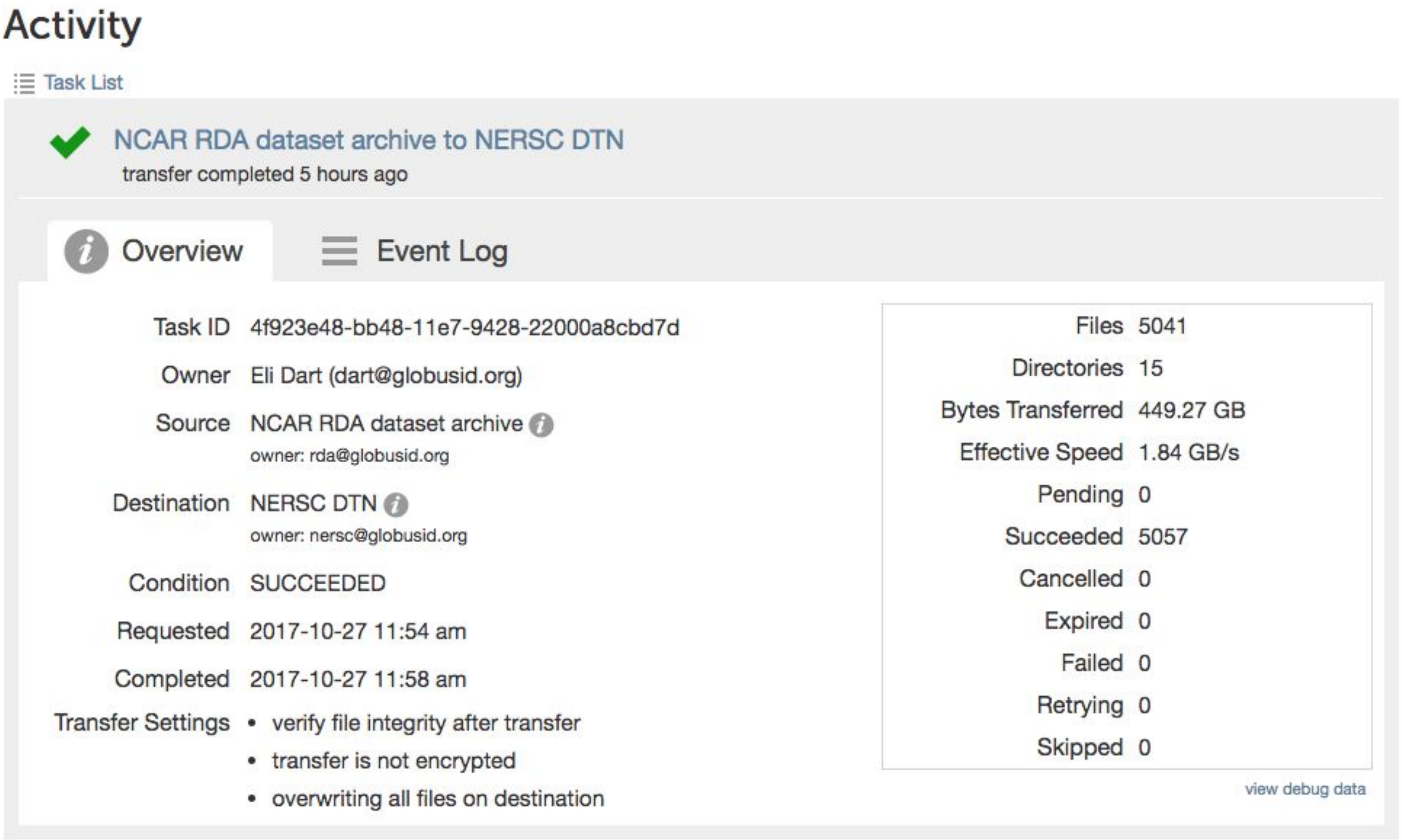
Transfer request submitted successfully. Task id: d2776d02-bb6f-11e7-9428-22000a8cbd7d ×

Endpoint: NCAR RDA dataset archive
Path: /ds313.0/

Endpoint: NERSC DTN
Path: /~/petascale-dtn/project/dtn/src/RDA/

1.9x2.5	Folder
index.html	258 B

Data Transfer from RDA Portal – Results



Activity

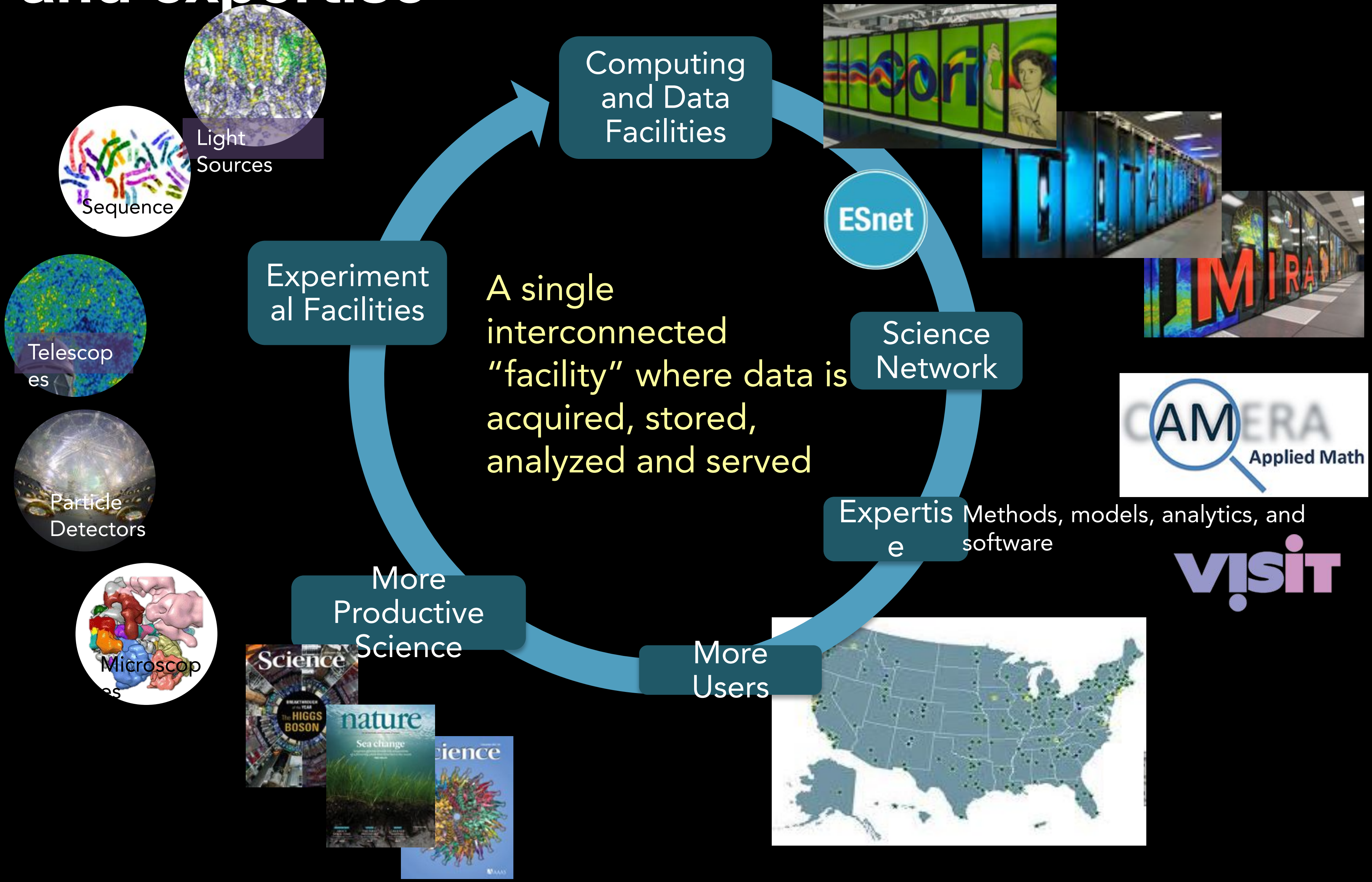
Task List

✓ NCAR RDA dataset archive to NERSC DTN
transfer completed 5 hours ago

Task ID	4f923e48-bb48-11e7-9428-22000a8cbd7d
Owner	Eli Dart (dart@globusid.org)
Source	NCAR RDA dataset archive owner: rda@globusid.org
Destination	NERSC DTN owner: nersc@globusid.org
Condition	SUCCEEDED
Requested	2017-10-27 11:54 am
Completed	2017-10-27 11:58 am
Transfer Settings	• verify file integrity after transfer • transfer is not encrypted • overwriting all files on destination

Files	5041
Directories	15
Bytes Transferred	449.27 GB
Effective Speed	1.84 GB/s
Pending	0
Succeeded	5057
Cancelled	0
Expired	0
Failed	0
Retrying	0
Skipped	0

Superfacility: integrated network of experimental and computational facilities and expertise



Light Sources

Sequence

Telescopes

Particle Detectors

Microscopes

Experimental Facilities

Computing and Data Facilities

Science Network

Expertise

More Users

More Productive Science

A single interconnected "facility" where data is acquired, stored, analyzed and served

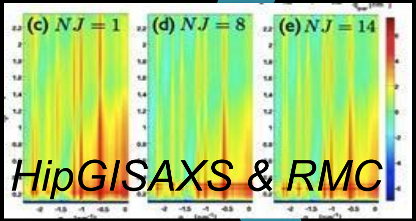
Methods, models, analytics, and software

Advanced Light Source Demonstration

ALS
ADVANCED LIGHT SOURCE

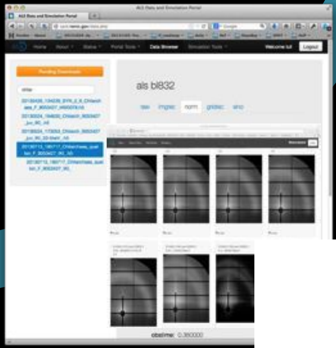
ESnet

GISAXS



HipGISAXS & RMC

CAMERA
Applied Math



Liu et al, "Fast printing and in situ morphology …". Adv Mater. 2015