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ENERGY SCIENCES NETWORK

The Science DMZ: Strategic Future

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U.S. DEPARTMENT OF
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Outline

- Science DMZ as a foundation
- New uses: Streaming DTNs
- Security: Science DMZ and Zero Trust

The Science DMZ as a Foundation

- At this point, there are many Science DMZ deployments
- Common use case: DTNs for file transfer
 - This is old hat or “normal” at this point, but it’s still important and valuable
 - Routine performance is enabling for science
- Wider deployment comes with network effects
 - Scientists can expect data transfer to work well
 - Good performance is becoming normalized, which means scientists can include it in their designs
- Growth beyond the simple case – more in a moment



The Value Of Routine Performance

- It's important to get to where high performance is normal
- No magic, no arcana, things just normally work – for petabytes of data
- DOE HPC facilities now easily shuffle around hundreds of terabytes
 - Some people have smaller data sets too
 - But the point is that it's normal and routine
- What follows is one specific example, chosen because of some specific features



[HOME](#) » [SITES](#) »

National Energy Research Scientific Computing Center

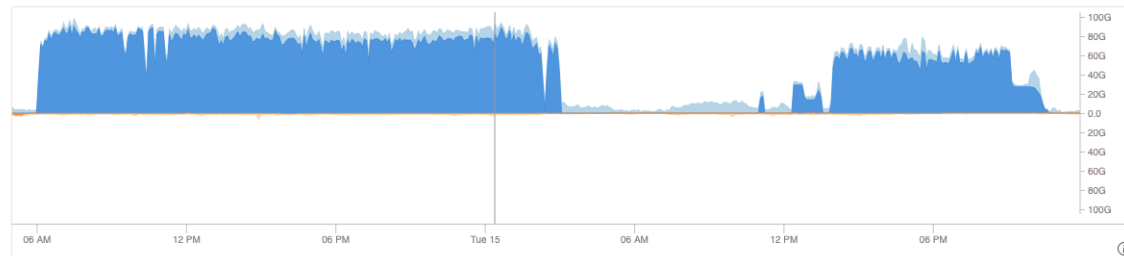
Website
<http://www.nersc.gov/>
[Interfaces](#)
[Flow](#)

 BREAKDOWN [Autonomous Systems \(origin\)](#) ▾

 TIME [day](#) [week](#) [month](#) [custom](#)

TOTAL SITE TRAFFIC

Tue Sep 15 12:24 AM 2020

 To site 81.6Gbps
 From site 2.49Gbps


TOP FLOWS BY AS_ORIGIN

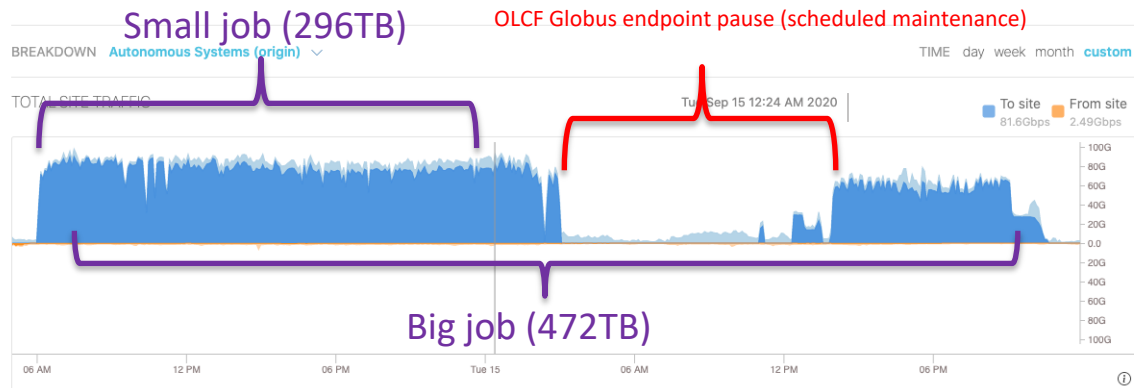
ORNL-MSRNET AS50	150Mbps	71Gbps
SLAC AS3671	9.2Mbps	5.6Gbps
FNAL AS3152	130Mbps	1.7Gbps
LBL AS16	1.4Gbps	2.2Gbps
SDSC AS195		
LANL-INET AS68	2.7kbps	
CIT AS31	1.6Mbps	580Mbps
UCB AS25	690Mbps	3.4Mbps
REDIRIS AS766	130Mbps	74Mbps
ARGONNE AS683	21kbps	260Mbps

National Energy Research Scientific Computing Center

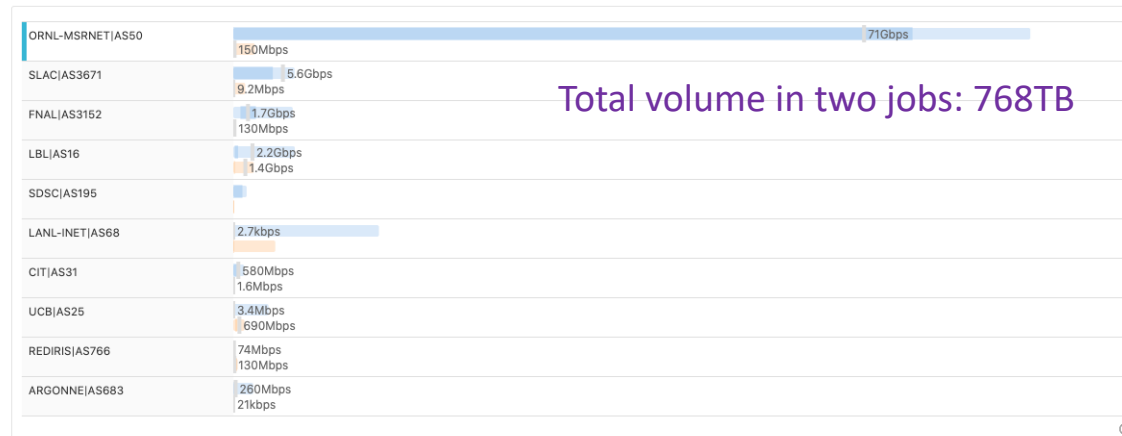
Website <http://www.nersc.gov/>

Interfaces

Flow



TOP FLOWS BY AS_ORIGIN



Key Points (1)

- Two Globus transfers from OLCF to NERSC were started by the same user (presumably for the same project – DESI – which is dark energy/cosmology) within 40 minutes of each other.
 - One transfer was ~350k files, ~296TB
 - Other transfer was ~1.8M files, ~472TB
 - Data transfer rate peaks over 80Gbps
 - Total transfer volume ~768TB
 - Total wall clock time ~39 hours
- Current tools (Filesystems, DTNs, Globus) handle petascale data sets easily



Key Points (2)

- Sophisticated tools bring multiple benefits
 - Both transfers experienced random data corruption (multiple checksum failures) which was automatically corrected by Globus (data set is $\frac{3}{4}$ of a petabyte....a lot can happen with that much data)
 - User had to expend zero effort to find and fix the corrupted files
 - OLCF endpoint paused for a workday for normal scheduled maintenance, and transfer resumed after maintenance concluded
 - OLCF staff did not have to worry about the user when planning maintenance
 - User had to expend zero effort to work around HPC facility maintenance
 - Easy to use tools with automated fault recovery reduce human effort
- Large scale data transfer is a key enabler for scientific productivity
 - Benefits of large-scale INCITE allocation brought back to collaborators
- Normal, routine operations – no magic

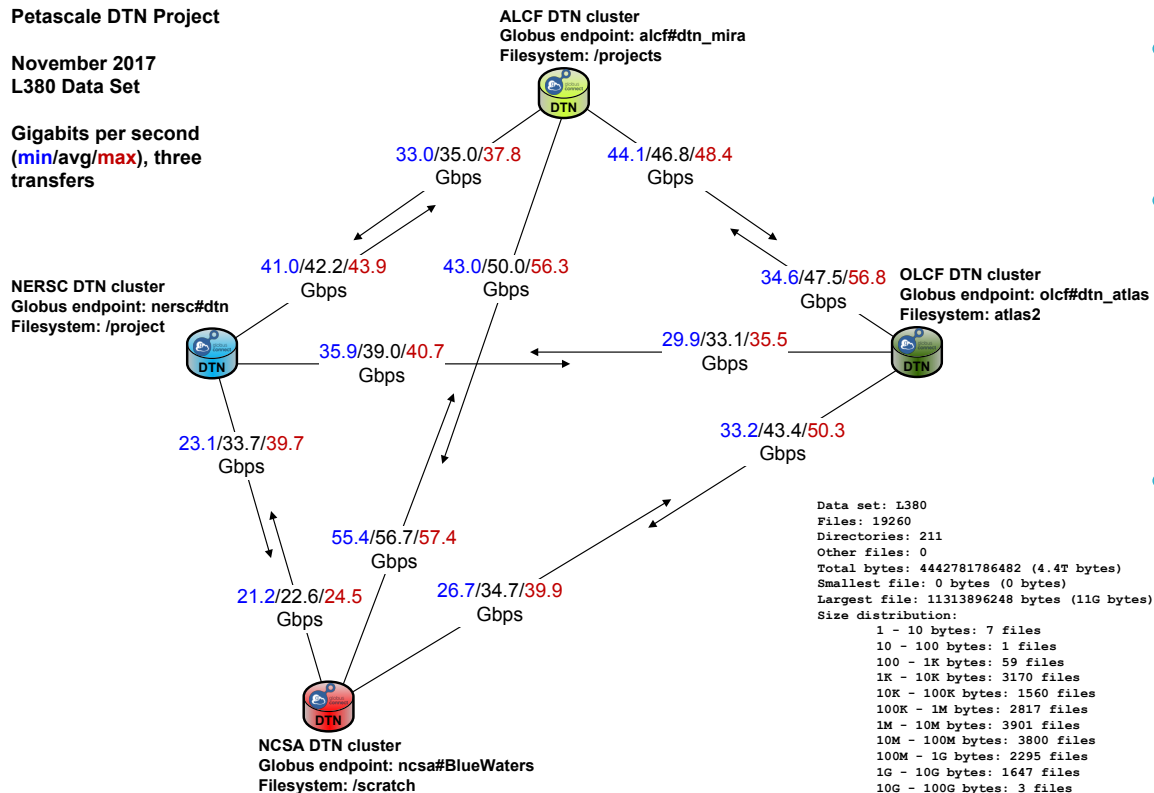


Petascale DTN Project – Durable Gains

Petascale DTN Project

November 2017
L380 Data Set

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

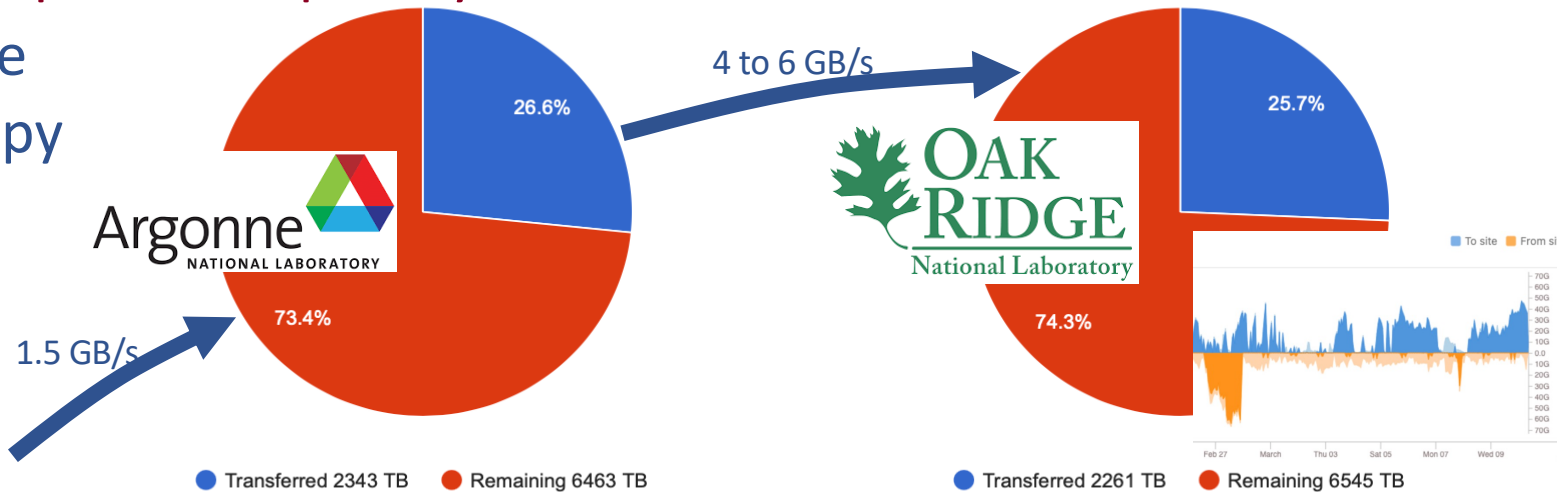


- Current performance 2x faster than 2017 numbers
- HPC facilities continue to maintain and improve capability because it is valuable to users
- Users now view this as normal, and can build new workflows on top of it



Challenge: Replicate 7+ petabytes of climate data to ANL and ORNL

Solution: Use Globus to copy data over ESnet



Replication to ALCF

ACTIVE, PAUSED and the latest SUCCEEDED transfers

No	Datasets	From	Requested	Completed	Status	Directories	Files	Bytes Transferred	Faults	Rate
1	/css03_data/CMIP6/CMIP/MOHC/HadGEM3-GC31-LL/historical	LLNL	2022-03-10 13:19:03		ACTIVE (20%)	6125	6515	6138646980430	0	832 MB/s
2	/css03_data/CMIP6/CMIP/MIROC/MIROC-ES2L/historical	LLNL	2022-03-10 05:35:04		ACTIVE (79%)	37994	409095	24611252181300	12	699 MB/s
3	/css03_data/CMIP6/CMIP/MOHC/HadGEM3-GC31-LL/amip	LLNL	2022-03-10 12:12:03	2022-03-10 13:18:06	SUCCEEDED	3908	1892	3091419704055	0	780 MB/s
4	/css03_data/CMIP6/CMIP/MOHC/HadGEM3-GC31-LL/abrupt-4xCO2	LLNL	2022-03-10 11:40:03	2022-03-10 12:11:57	SUCCEEDED	1121	953	1559216858805	0	814 MB/s

Replication to ORNL

ACTIVE, PAUSED and the latest SUCCEEDED transfers

No	Datasets	From	Requested	Completed	Status	Directories	Files	Bytes Transferred	Faults	Rate
1	/css03_data/CMIP6/CMIP/MIROC/MIROC-ES2L/esm-piControl	ALCF	2022-03-10 15:14:03		ACTIVE (25%)	1236	40039	1407934487539	0	2.93 GB/s
2	/css03_data/CMIP6/CMIP/IPSL/IPSL-CM6A-LR/historical	ALCF	2022-03-09 22:02:03		ACTIVE (77%)	73193	36610	129503497305534	1	2.08 GB/s
3	/css03_data/CMIP6/CMIP/MIROC/MIROC-ES2L/esm-hist	ALCF	2022-03-10 14:51:04	2022-03-10 15:13:24	SUCCEEDED	3706	39663	2973432261868	0	2.22 GB/s
4	/css03_data/CMIP6/CMIP/MIROC/MIROC-ES2L/amip	ALCF	2022-03-10 14:47:03	2022-03-10 14:50:22	SUCCEEDED	3126	12284	446324011629	0	2.25 GB/s

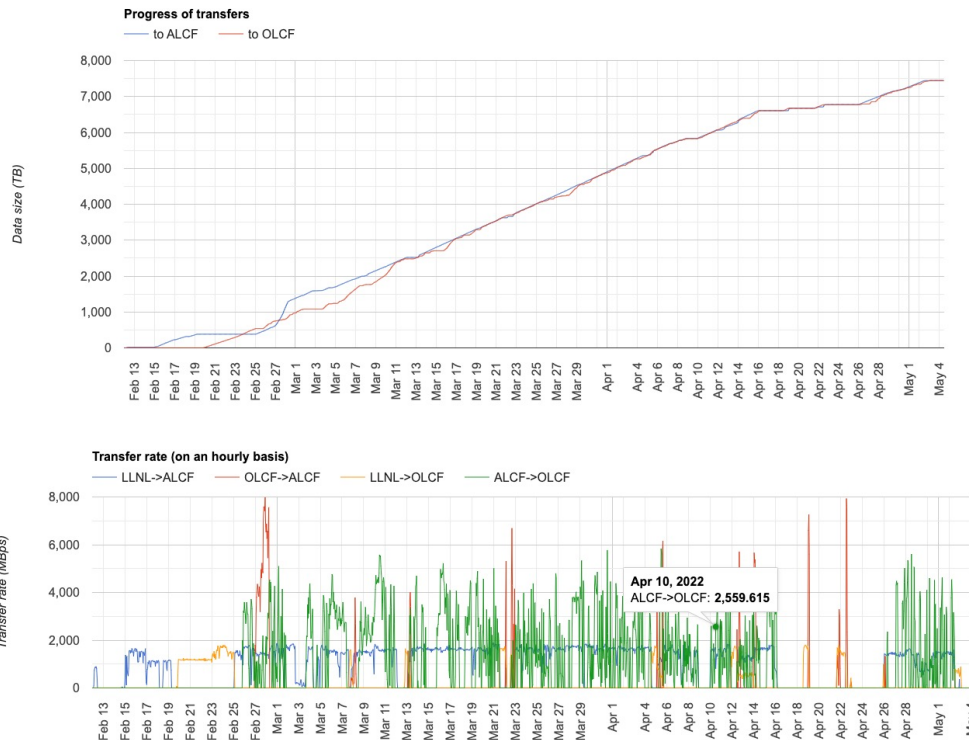
<https://dashboard.globus.org/esgf>

Slide credit: Ian Foster, ANL

As of March 10, 2022

Climate Data Replication

- Transfers mostly LLNL→ANL→ORNL except during maintenance windows
- Overall end2end performance limited on LLNL side
 - Storage system config
 - Keep that one working, sync between the other two
- This is a good reason to deploy capable DTNs and storage systems
 - Technical capabilities define the boundaries of the possible
 - If your users can't reason about something, they won't ask you for it



<https://dashboard.globus.org/esgf>



Data Portals Increasing Adoption

Datasets

Choose the dataset(s) you wish to download, then click the **Transfer** button to begin transferring the full dataset(s) from NERSC. Or, you can click on a catalog dataset to browse and choose individual files for transfer (not supported for image datasets). See [here](#) for detailed instructions.

To learn more about a dataset, click the "doc" link next to the dataset name.

Dataset filter: ☒ Catalogs ☐ Images ☐ Deprecated

Dataset Name	Size	Select
DC2 Truth Match dr6 v4 (doc)	52 GB	<input type="checkbox"/>
DC2 Unmerged Truth Star (for release v4) (doc)	59 GB	<input type="checkbox"/>
DC2 Unmerged Truth SN (for release v4) (doc)	2.2 GB	<input type="checkbox"/>
DC2 Unmerged Truth Galaxy (for release v4) (doc)	68 GB	<input type="checkbox"/>
DC2 Object DP2D dr6 v4 (doc)	118 GB	<input type="checkbox"/>
DC2 Raw Image dr6 v4 (2 tracts) (doc)	932 GB	<input type="checkbox"/>
DC2 Raw Image dr6 v4 (2 patches) (doc)	74 GB	<input type="checkbox"/>
DC2 Calibrated Exposure dr6 v4 (2 tracts) (doc)	5.4 TB	<input type="checkbox"/>
DC2 Calibrated Exposure dr6 v4 (2 patches) (doc)	495 GB	<input type="checkbox"/>

Datasets

Choose the dataset(s) you wish to download, then click the **Transfer** button to begin transferring the full dataset(s) from NERSC. Or, you can click on a catalog dataset to browse and choose individual files for transfer (not supported for image datasets). See [here](#) for detailed instructions.

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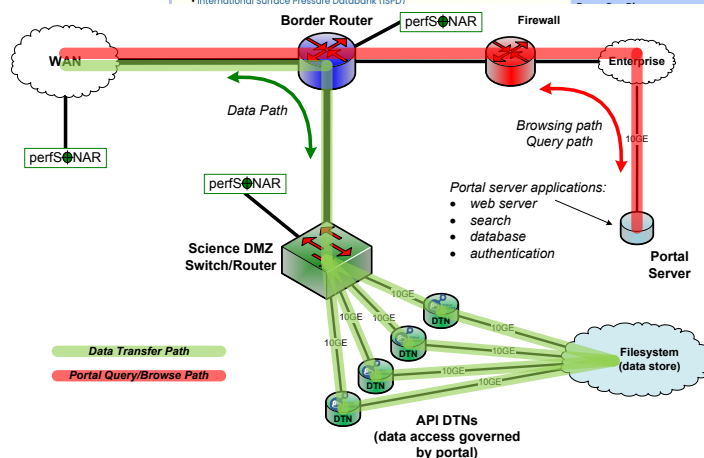
Permissions filter: ☒ Public ☒ CMB-S4 ☐ CMB-S4 DM

Dataset filter: ☒ Design tool simulations 1 (DT1) ☒ Data Challenge 1 (DC1)

☐ Deprecated

Dataset Name	Size	Select
DT1_Lensed CMB scalar only (doc)	30 GB	<input type="checkbox"/>
DT1_CMB tensor only r3e3e3 (doc)	30 GB	<input type="checkbox"/>
DT1_Noise only no splits (doc)	31 GB	<input type="checkbox"/>
DT1_Noise + Atmosphere, full and 7 splits, LAT Chile (doc)	172 GB	<input type="checkbox"/>
DT1_Noise + Atmosphere, full and 7 splits, LAT Pole (doc)	200 GB	<input type="checkbox"/>
DT1_Noise + Atmosphere, full and 7 splits, SAT Pole (doc)	121 GB	<input type="checkbox"/>
DC1_CMB Cosmological maps LAT Chile (doc)	221 GB	<input type="checkbox"/>

Transfer



Data from Mira-TitanU Snapshots

The Mira-Titan Universe simulation suite was carried out on Mira, a supercomputer at the Argonne Leadership Computing Facility, and Titan, at the Oak Ridge National Laboratory. The simulations cover a range of cosmological models including models with a dynamical dark energy equation of state parameterized via w_0 and w_a . Each simulation covers a $(2.16 \text{ Gpc})^3$ volume and evolves 3200³ particles. We provide outputs for 27 redshifts, between $z=4$ and $z=0$, including halo information and down-sampled particle information.

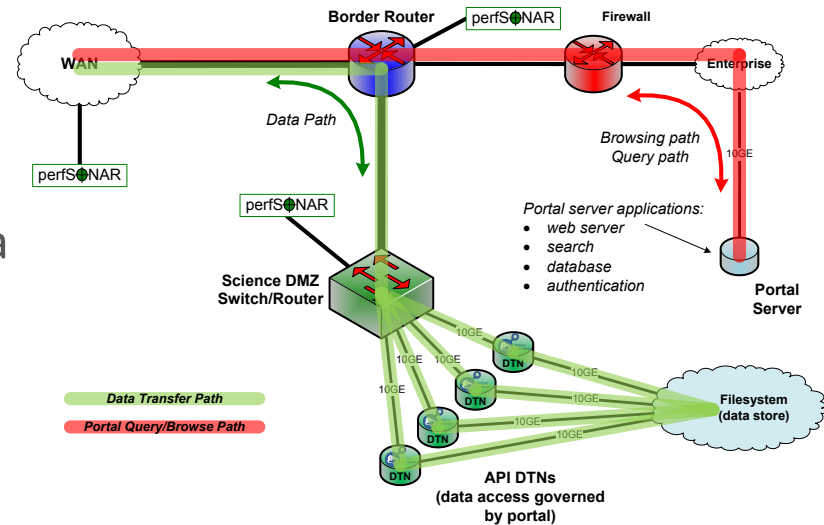
Please select one or more models from the list below, then select all the relevant redshifts and data products. The Submit/Transfer button will indicate the number and overall size of the selected files that you aim to transfer. This button will lead you to the Globus interface. The search box at the top allows you to narrow the model selection by specifying a model number or a numerical value for any cosmological parameter.

Model	Ω_m	Ω_b	Ω_c	h	σ_8	n_s	w_0	w_a
M000	0.2200	0.02238	0.0	0.7100	0.8000	0.9630	-1.0000	0.0000
M001	0.3276	0.02261	0.0	0.6167	0.8778	0.9611	-0.7000	0.6722
M002	0.1997	0.02328	0.0	0.7500	0.8556	1.0500	-1.0330	0.9111
M003	0.2590	0.02194	0.0	0.7167	0.9000	0.8944	-1.1000	-0.2833
M004	0.2971	0.02283	0.0	0.5833	0.7889	0.8722	-1.1670	1.1500



Data Portals Increasing Adoption

- Data publication and access built on the Science DMZ foundation
- Multiple fields: Astronomy, Cosmology, Genomics, Climate
- Science DMZ and DTNs support data search, publication, access
- Typically classical file-based access, but important to scientific communities for navigating large repositories

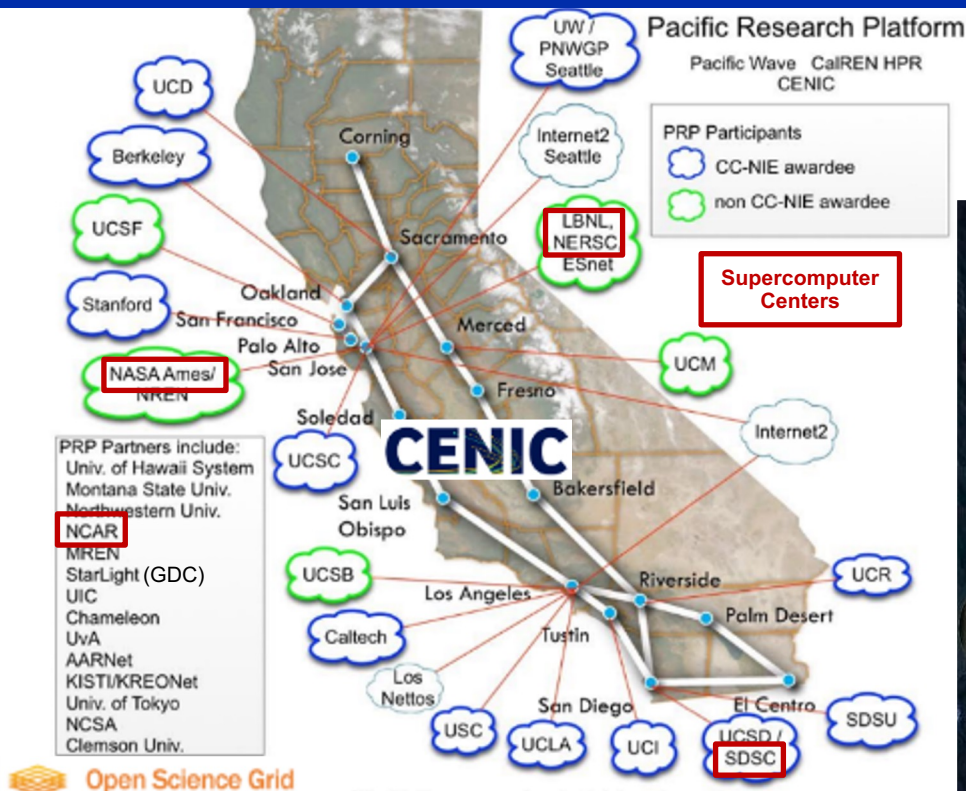


Integrating Many Science DMZs

- Instead of building one Science DMZ for one service, some communities have built one service from many Science DMZs
- Use the DMZ and a DTN as a building block
 - Many DTNs working together result in a distributed capability
 - Higher-layer software stack may be more than just data transfer
- Example: PRP and NRP
 - DTN + GPUs
 - Data-centric distributed computing capability



2015 Vision: The Pacific Research Platform Will Connect Science DMZs Creating a Regional End-to-End Science-Driven Community Cyberinfrastructure



NSF CC*DNI Grant
\$7.3M 10/2015-10/2020



Note: this diagram represents a subset of sites and connections.

Open Science Grid

PRP
 PACIFIC RESEARCH
 PLATFORM

Source: John Hess, CENIC

PRP
 PACIFIC RESEARCH
 PLATFORM

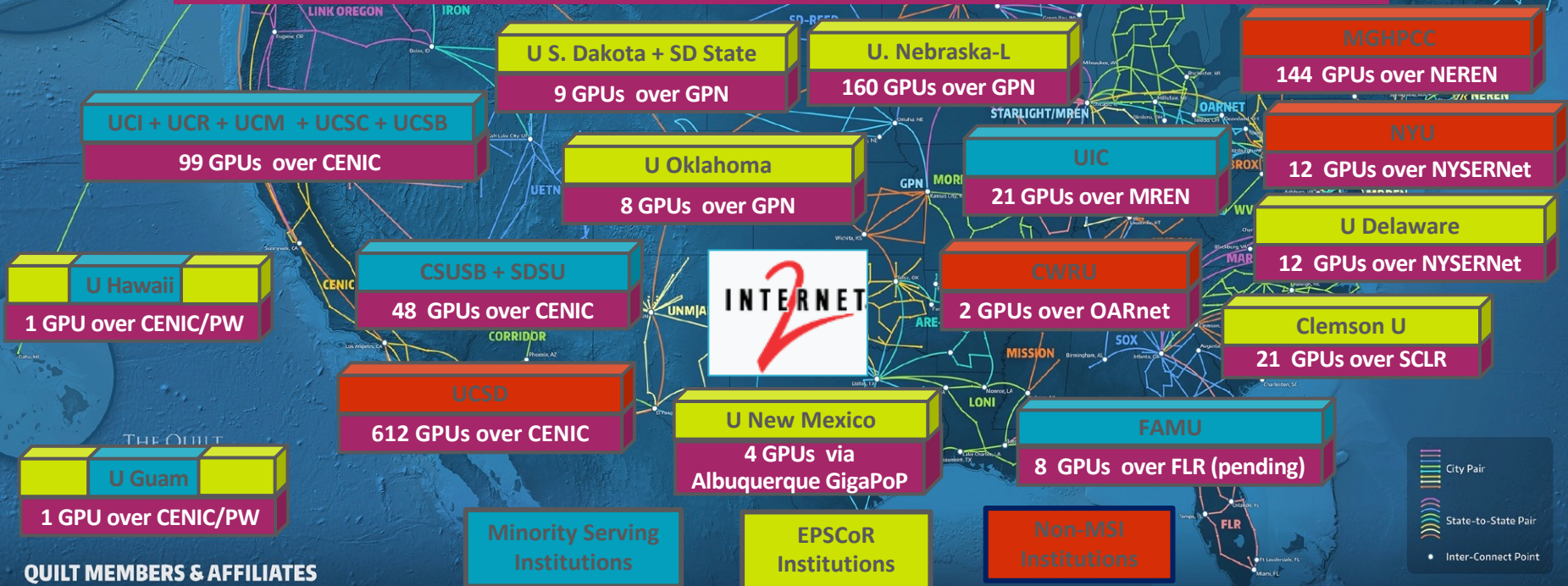
CITRIS
 BANATAO
 INSTITUTE

SDSC

it²

Nautilus ~1,100 GPUs Distributed over US Networks—Fall 2022

(New: NSF PNRP's 352 GPUs, and ARO/DURIP's 144 GPUs and SDSU's 4 DGX A100s)



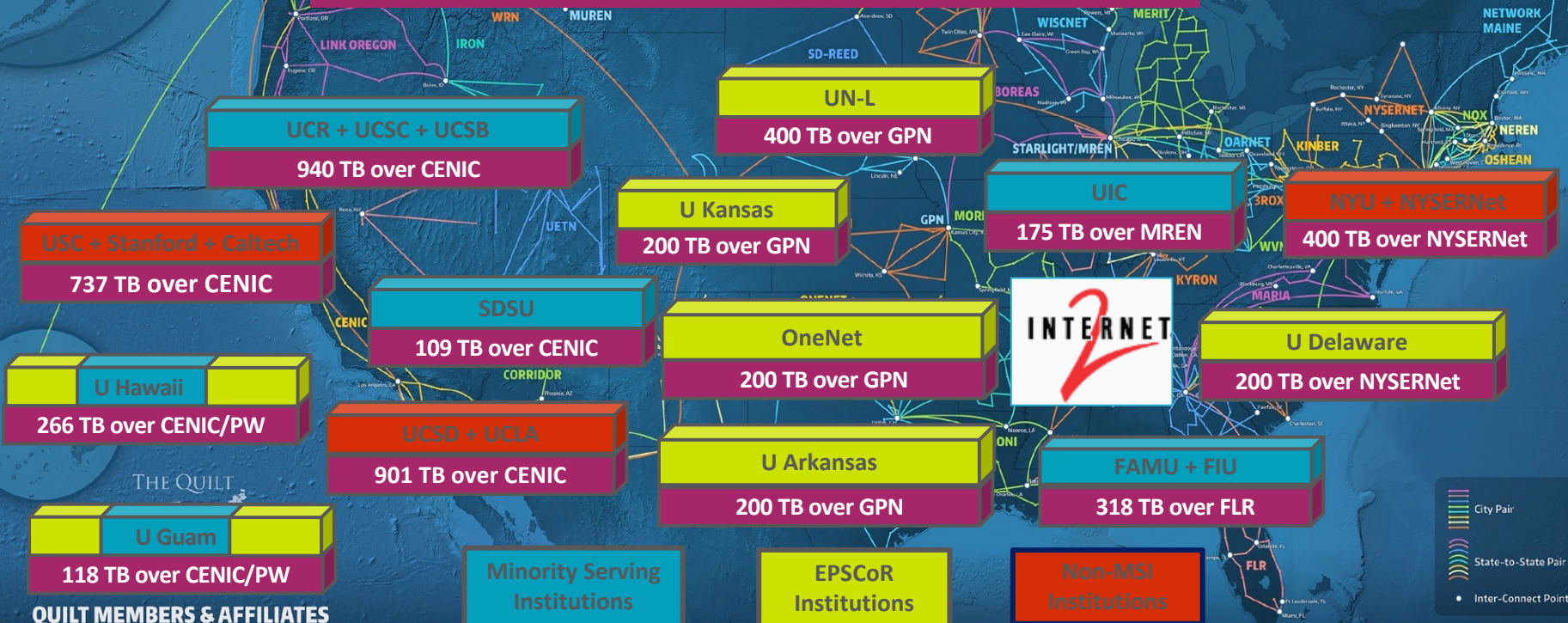
QUILT MEMBERS & AFFILIATES



Slide Credit:

Tom DeFanti, UCSD

5 PB Nautilus Ceph Storage Over Networks—2022



QUILT MEMBERS & AFFILIATES

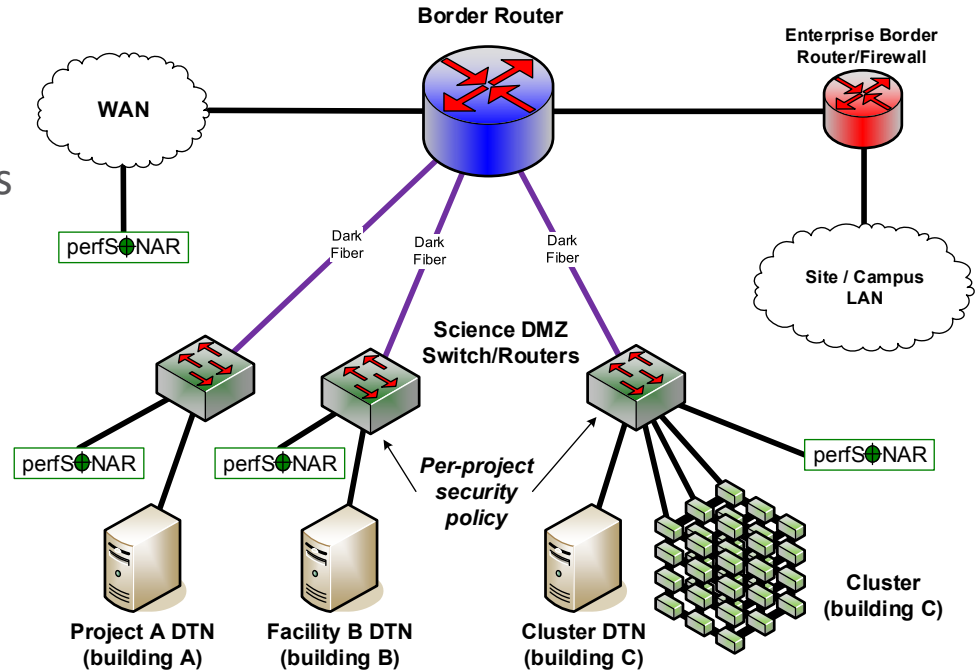
Streaming DTNs: Near Real Time Data Processing

- File movement is great for many applications, but not all
 - Fast feedback for experiment guidance
 - Integration of detectors and computing
- In some cases, filesystem I/O is too slow
- In other cases, file semantics aren't a good fit
 - Message passing is more appropriate in some workflows
 - Files may be present in the workflow, but only after a streaming pipeline



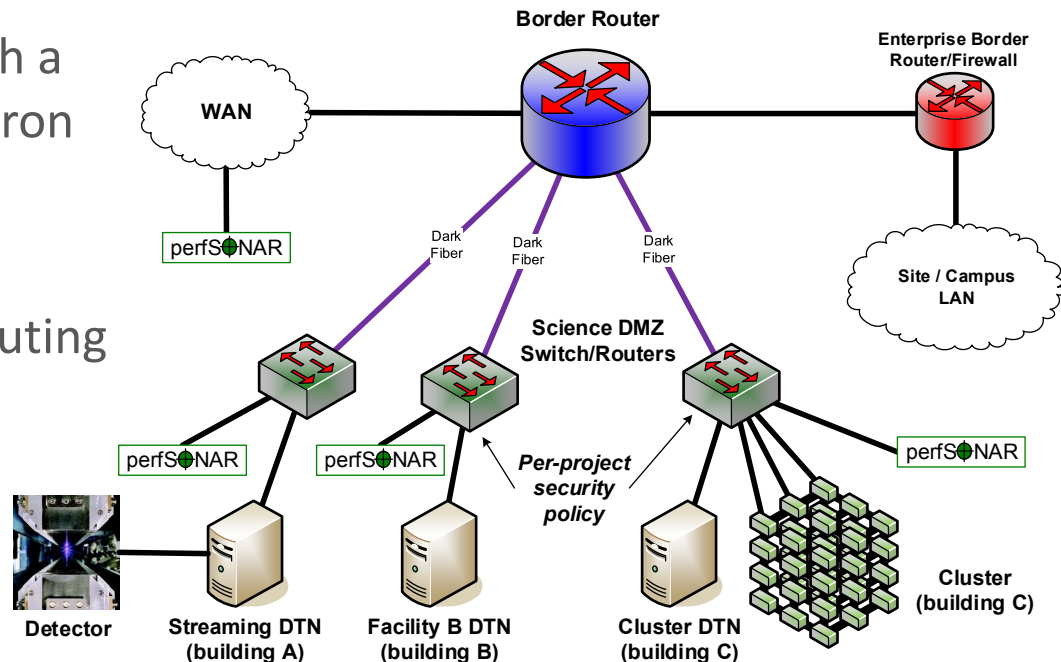
Streaming DTN – Just Another Flavor

- In many cases, a DTN is deployed to support file transfer
 - Large data sets between filesystems
 - Well-understood workflow
- Can have many DTNs in a single Science DMZ, or multiple Science DMZs as appropriate
- Let's put Project A at an experimental facility



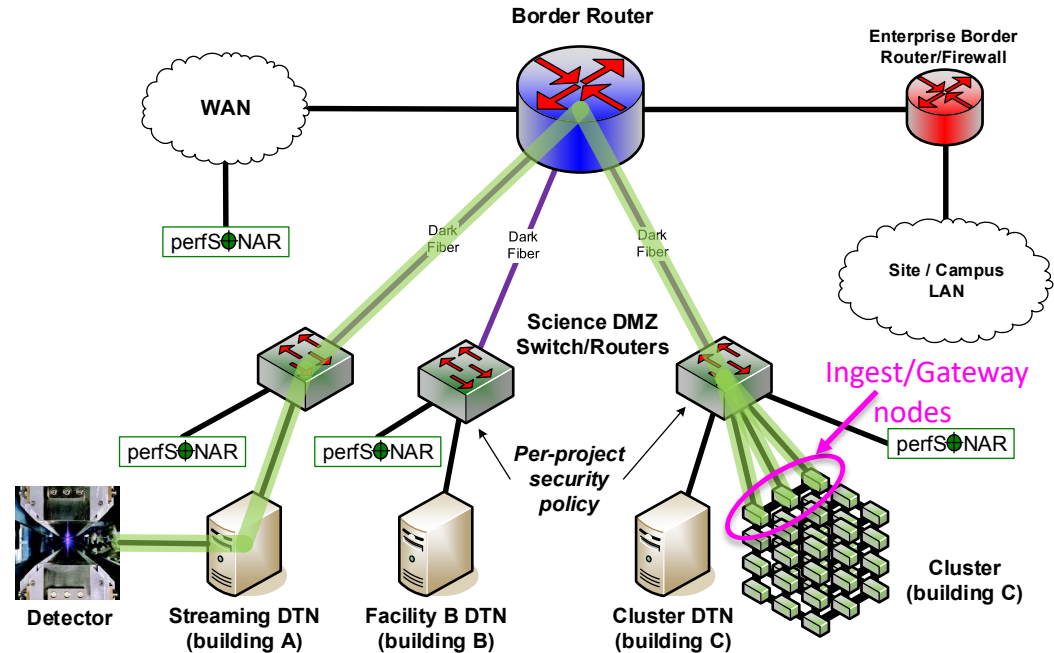
Common Case – DAQ for a Detector

- Project A is an experiment with a high-speed detector (synchrotron light source, Cryo-EM, etc.)
- Rapid analysis for experiment feedback requires more computing than can be deployed at the experiment
- Stream the data to remote compute resource



Streaming Data Path

- High performance data path requires consistent behavior, low packet loss, etc.
- Perfect fit for Science DMZ performance engineering
- Stream to local or remote computing depending on application
 - (local shown here because it all fits in one diagram)



Stream Processing in Light Source Facilities

A Science Driver

Experiment



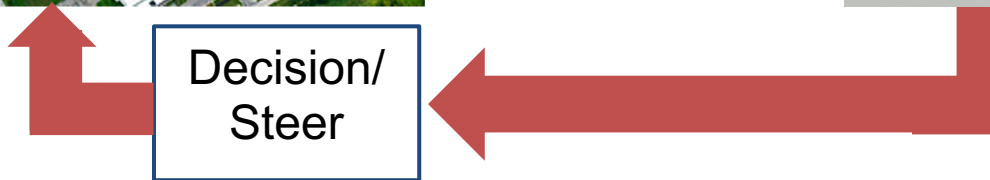
Transfer data



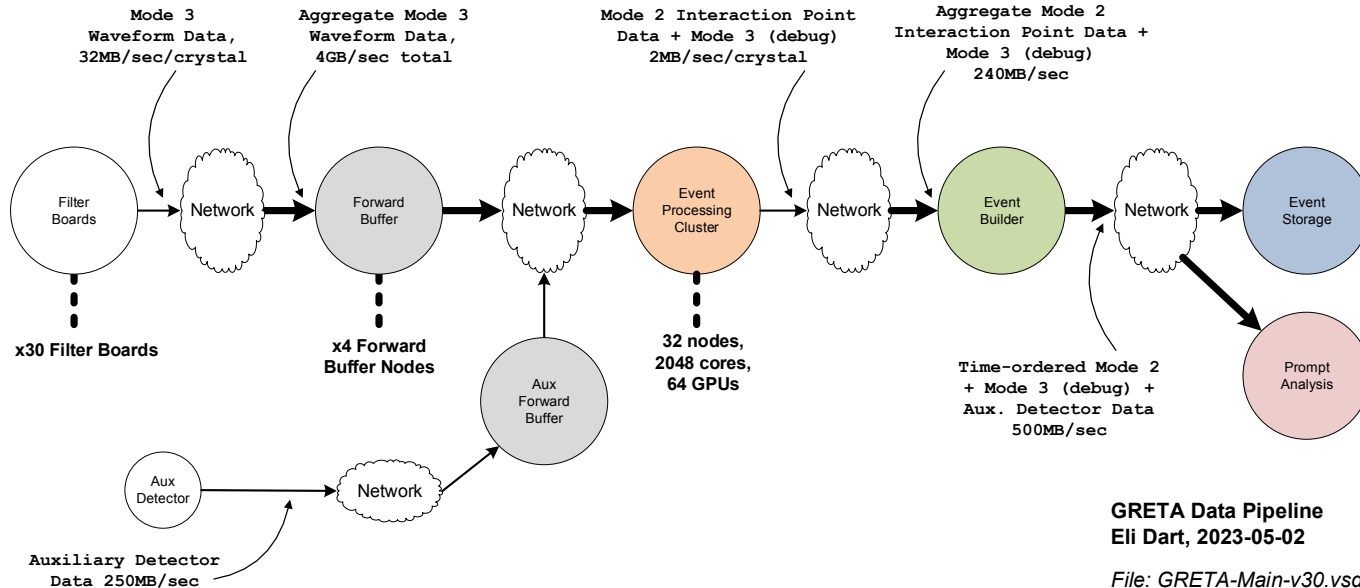
Data Analysis



Decision/
Steer

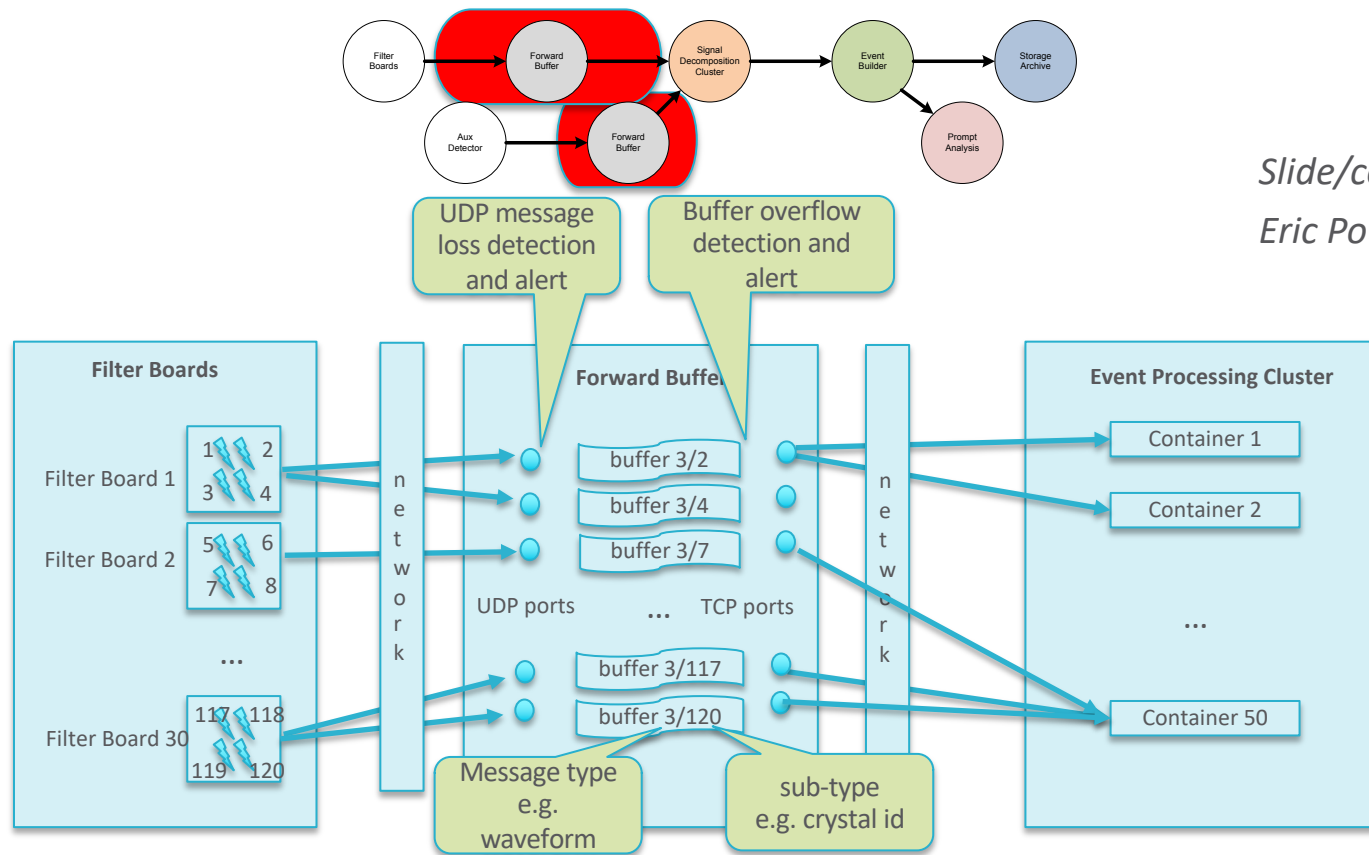


GRETA Computing/Data Pipeline



- Abstract depiction of computing pipeline, including device counts and data rates
- Computing pipeline serves as a platform for data processing, from detector electronics on the left to visualization and storage on the right

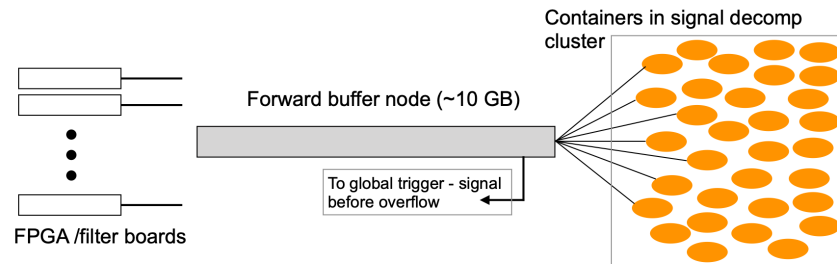
Forward Buffer Architecture



Slide/code credit:
Eric Pouyoul, ESnet

Forward Buffer Design Pattern

- Generalized forward buffer design under development
- Use GRETA pipeline as a starting point, remove GRETA-specific aspects
- Goal: re-usable code to couple UDP detector readout to self scheduling inline computing



Forward buffer performance: see *Simple and Scalable Streaming: The GRETA Data Pipeline*, EPJ Web of Conferences 251, 04018 (2021)

Message size	Maximum message rate (Single stream)	Maximum streams at 20k messages / sec
100 bytes	≥ 400k*	50
500 bytes	≥ 400k*	50
1 kB	270k	50
5 kB	210k	50
8 kB	172k	50
8.8 kB	170k	50
9.2 kB	110k	20
20 kB	80k	18
40 kB	50k	16
64 kB	28k	*

Streaming DTNs

- There are more applications of streaming DTNs
 - FPGA-based devices to distribute detector output to computing (EJFAT)
 - More to come, I'm sure
- Need Science DMZ capabilities
 - High bandwidth
 - Specific security
- Difficult to deploy and operate in an environment without Science DMZ

Science DMZ Security

- Goal – disentangle security policy and enforcement for science flows from security for business systems
- Rationale
 - Science data traffic is simple from a security perspective
 - Narrow application set on Science DMZ
 - Traditional perimeter security is a poor fit for high performance flows
- Separation allows each to be optimized
 - Key point: the Science DMZ is an example of segmentation for a specific purpose, and with specific security policy
 - Separate Science DMZ from the perimeter for security and performance reasons



Zero Trust – The Demise Of The Perimeter

- No implied trust based on network location
 - “Network location” means IP address and physical topology
 - “Inside the firewall” does not confer additional trust
- Access control is as granular as possible
 - “Bulk” security at the perimeter → per-service policy + filter
 - Policy enforcement close (in topology) to running service
 - Focus on authn, authz, reducing zones of implied trust
- What does this mean for Science DMZ?

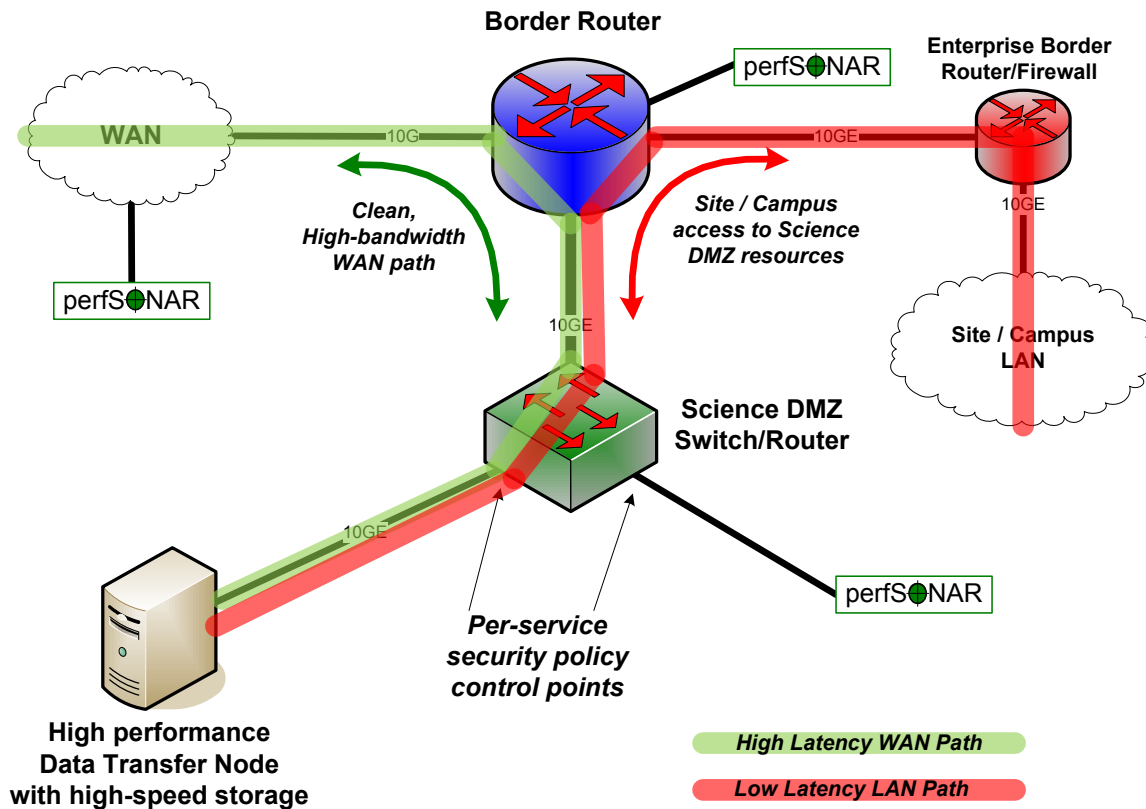


Zero Trust Elements

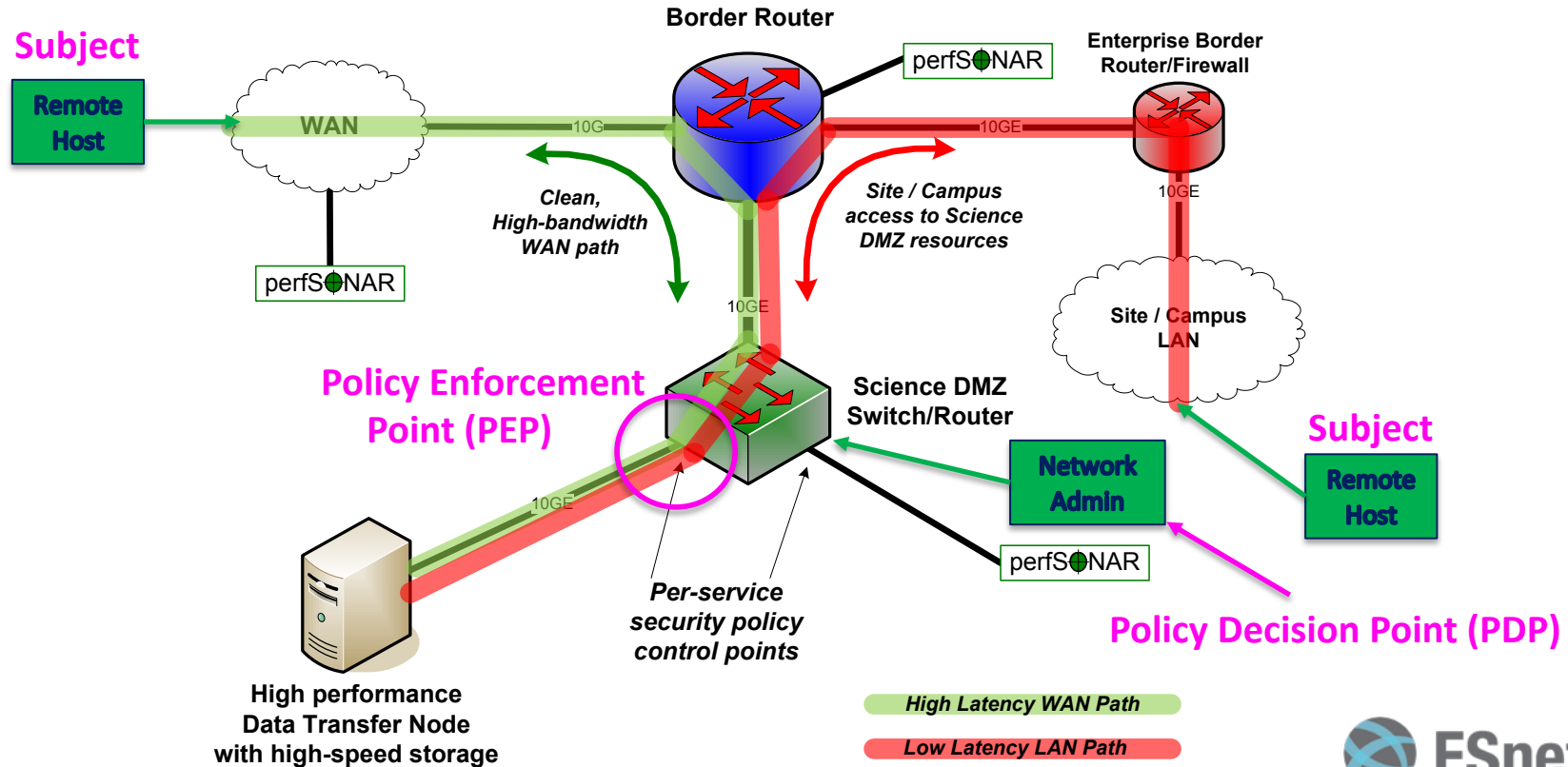
- Multiple information sources
 - NIST 800-207
 - CISA Zero Trust Maturity Model
 - Others
- A Subject accesses a Resource
 - Permission granted (or not) by Policy Decision Point (PDP)
 - Policy Engine
 - Policy Administrator
 - Policy is enforced by Policy Enforcement Point (PEP)
 - Path between Subject and PEP is untrusted
 - Path between PEP and Resource is trusted
- Micro-segmentation, per-session authentication are key ideas



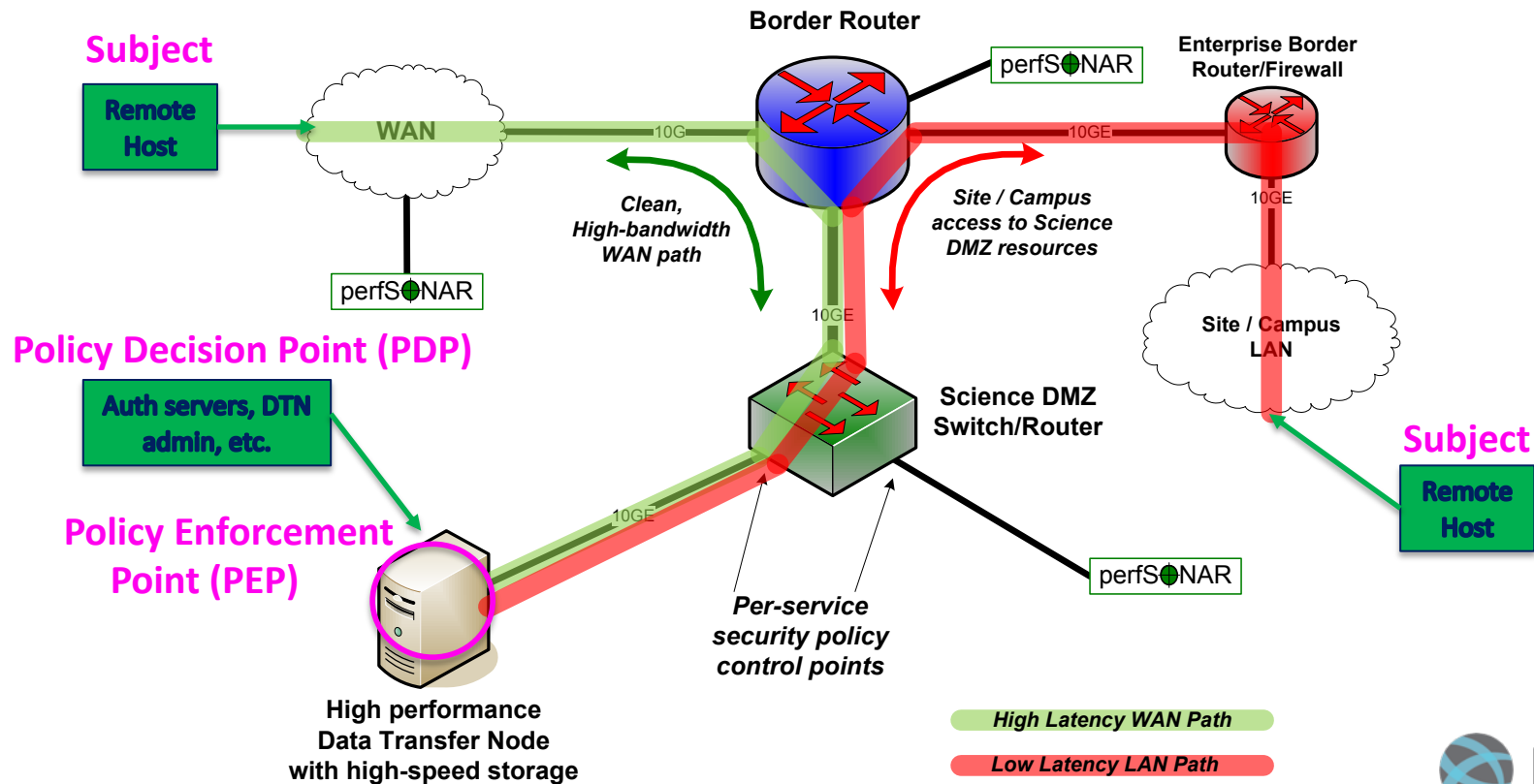
Science DMZ With Zero Trust Labeling



Science DMZ With Zero Trust Labeling – Network Layer



Science DMZ With Zero Trust Labeling – Application Layer



Zero Trust – Segmentation Matters

- The Science DMZ model already brings security policy enforcement close to the service
 - For example, we put DTN filters on the Science DMZ switch or router if possible, not at the perimeter
 - Segmentation by function is relevant to both security and performance
 - Micro-segmentation is a good fit for Science DMZ (and we do this already)
- Network layer filters are still relevant, even as more focus is given to the application
 - Layer 3 filter is a network-layer policy decision on what remote hosts to serve
 - Layer 4 filter is a network-layer policy decision on permitted DTN services
 - Most of Zero Trust works at the application layer (users, roles, data, etc)



Zero Trust and Science DMZ

- Transition to Zero Trust will affect DTN applications more than DMZ networks
 - Science DMZ itself is important for performance and security
 - Application stack needs modern authn, authz
 - Affects application choices and configuration
 - Performance requirements are unaffected by auth mechanisms
- Topology is important for performance
 - Data plane capabilities, reduction of complexity, etc.
 - Important to retain data plane improvements as we improve application and data security using Zero Trust
- Science DMZ is inherently Zero Trust compatible
- Iterative deployment/improvement is still key



Science DMZ – Moving Forward

- The Science DMZ is part of the data ecosystem
- Solid foundation for building higher-level services and capabilities
 - Many communities have made it their own
 - Keep what you need, add new things, whatever works for the science
- File-based workflows continue to be important
 - Data transfer
 - Data portals
- Streaming is a new and growing area
- Zero Trust is changing security – Science DMZ is a good fit





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Thanks!

Energy Sciences Network (ESnet)

Lawrence Berkeley National Laboratory

<http://fasterdata.es.net/>

<http://my.es.net/>

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