The CI Landscape: Systems, Service Providers, Technologies

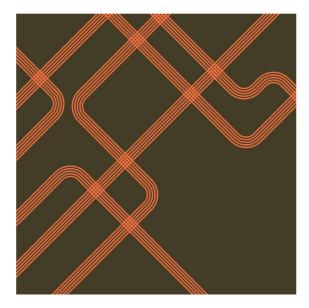
Jacob Fosso Tande,

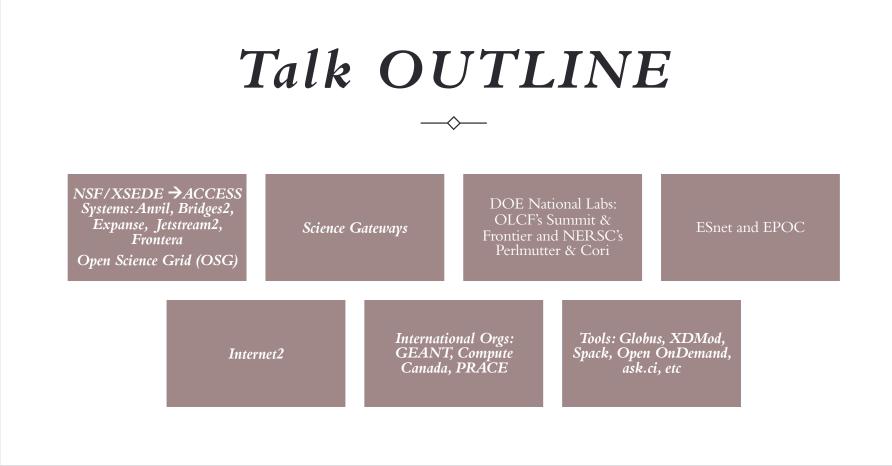
The University of North Carolina at Greensboro,

Campus Champions Leadership Team,

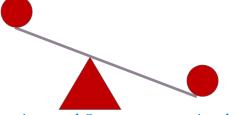
Virtual Residency

June 28, 2022





Striking the Right Balance



Services and Systems are omitted because of:

- 1. Expanded landscape
- 2. Time
- 3. Where to find?

The following are omitted:

- NSF/ACCESS: Darwin, Rockfish, Open Storage Network(OSN), Stampede2, FASTER
- DOE National Lab resources such as the ALCF's Aurora & Polaris test bed.
- NIH resources such as BioWulf, Helix and Helixweb
- Cloud resources such as CloudBank, CloudLab, GENI, emulab and Chameleon.
- Commercial Cloud: Google Cloud, Azure, AWS, IBM cloud etc..
- Regional Networks and THE QUILT

Why Bother?

• You are from a resource limited institution.

• Your users have needs that are not present at your institution.

○ Extreme memory compute systems

Testbeds

o Distributed data sharing (Open Storage Network)

0 Demand surpasses offer

Highly collaborative research projects:

IceCube project

Event Horizon Telescope Collaboration

What is more important? Knowing all about the systems and services or knowing where to find these systems and services?

NSF/XSEDE →ACCESS Systems Startup Allocations

Why get a Startup Allocation?

- Small-scale computational activities that require the unique capabilities of resources allocated through XSEDE
- Application development by researchers and research teams
- Benchmarking, evaluation and experimentation.
- Developing a science gateway or other infrastructure software components



NSF/XSEDE →ACCESS Systems Startup Allocations

Share your thoughts in the chat: If you have/had a startup allocation, how do/would you use it?

Anvil HPC



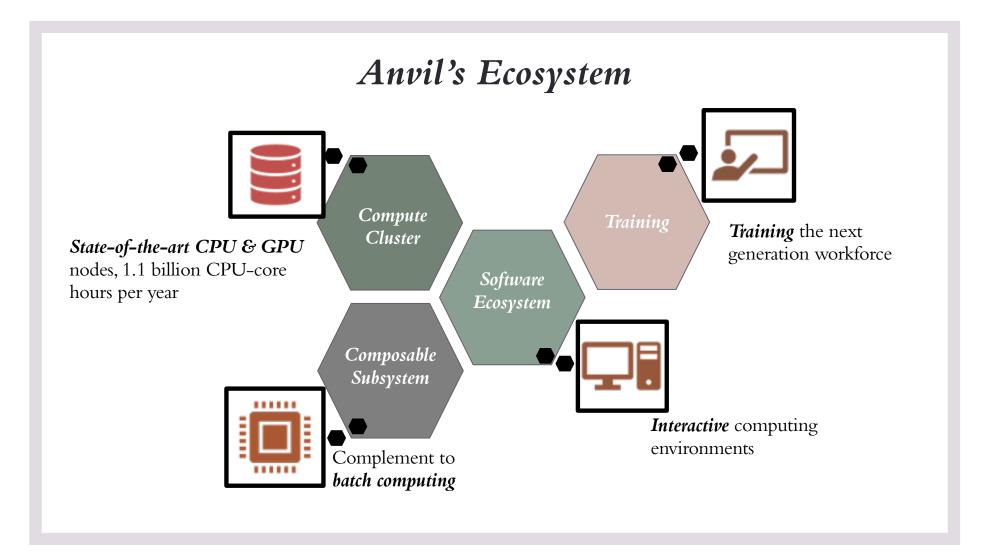
"... reflects the Purdue Boilermakers' strength and workmanlike focus on producing results ..."

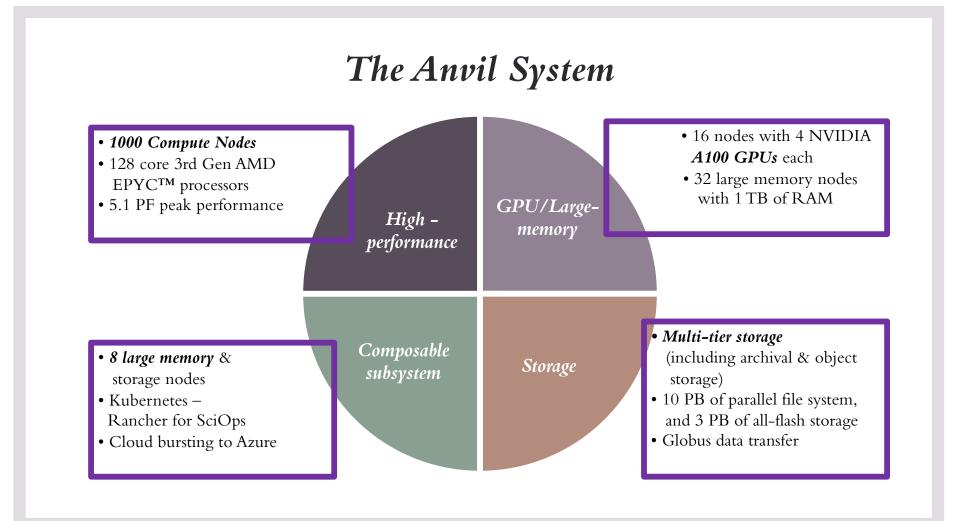
C a t e g o r y *I* : A National Composable

Advanced Computational Resource for the Future of Science and Engineering

5-year Production Operations

Started Feb 2022





The Anvil Software Stack

| Programming Libraries and Compilers | Various popular programming languages, GNU, Intel and AOCC compilers, message passing libraries Workflow and data management and analysis tools Debugging and profiling tools |
|---|--|
| Scientific Applications | General purpose mathematics and statistics modeling tools, numerical libraries, visualization tools Broad application base with installs and modules from various science and engineering domains |
| Containers and Datasets | Support for Singularity containerization and execution Efficient access to various databases (e.g., NCBI) |

Bridges-2 HPC



Provides transformative capability for rapidly evolving, computation-intensive and data-intensive research, creating opportunities for collaboration and convergence research.

Connecting new communities to advanced research computing.

Latest AMD EPYC processors

Approximately 3x larger than Bridges

Fast flash array and tiered data management

Interoperability with cloud and campus resources

Designed for Full System AI and data-centric computing

| | More Science: |
|------|-------------------|
| 1200 | Faster Computing: |
| - 1 | Faster Storage: |
| | Smarter Science: |
| | Scalable: |

"PSC's newest supercomputer"

Carnegie Mellon University



Bridge-2's Concepts

Bridges-2 core concepts:

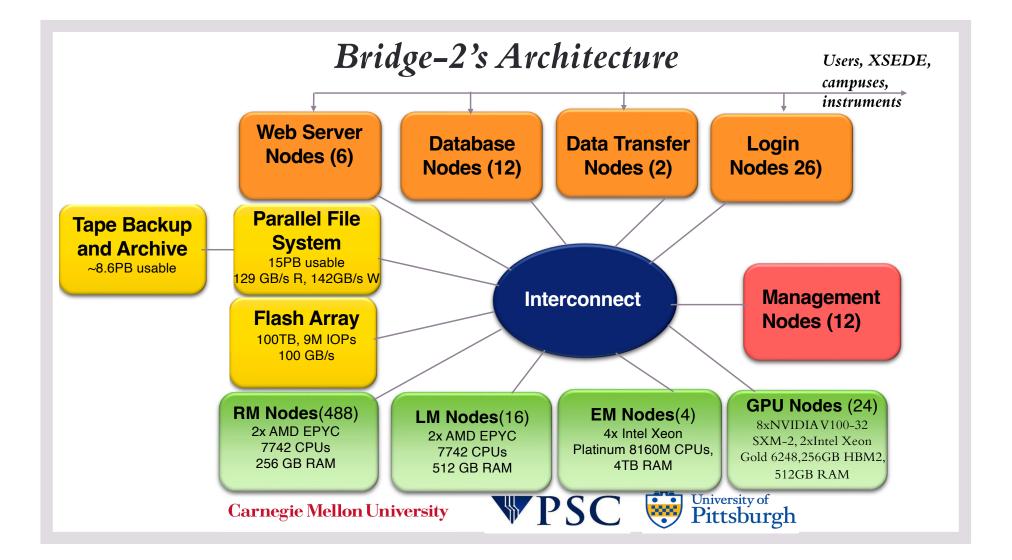
- Converged HPC + AI + Data
- Custom fat tree Clos topology optimized for datacentric HPC, AI, and HPDA
- Heterogeneous node types for different aspects of workflows
- CPUs and AI-targeted GPUs
- 3 tiers of per-node RAM (256GB, 512GB, 4TB)
- Extremely flexible software environment
- Community data collections & Big Data as a Service

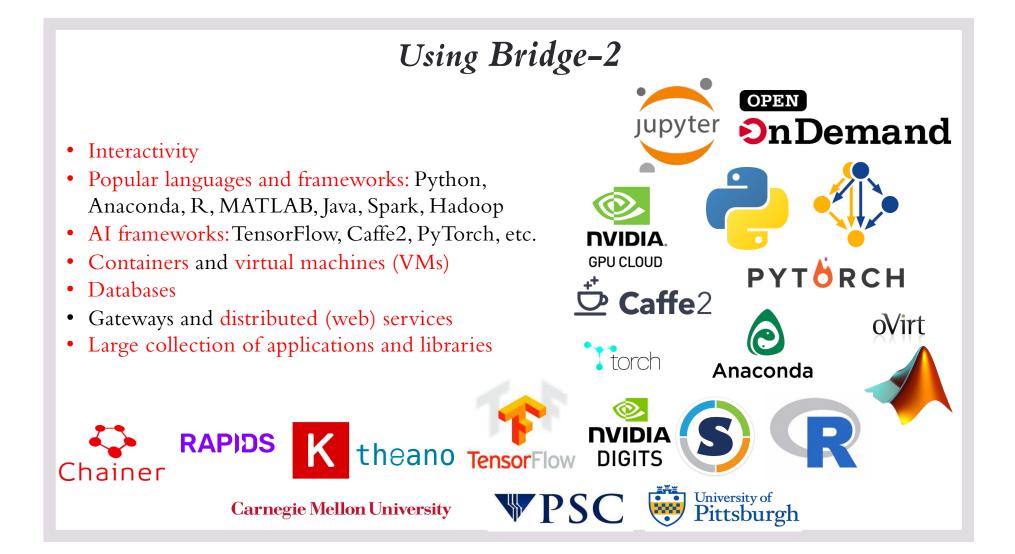
Innovations beyond Bridges:

- AMD EPYC 7742 CPUs: 64-core, 2.25-3.4 GHz
- AI scaling to 192V100-32GB SXM2 GPUs
- 100TB, 9M IOPs flash array accelerates deep learning training, genomics, and other applications
- Mellanox HDR-200 InfiniBand doubles bandwidth &supports in-network MPI-Direct, RDMA, GPU Direct, SR-IOV, and data encryption
- Cray ClusterStor E1000 Storage System
- HPE DMF single namespace across disk and tape for data security and expandable archiving

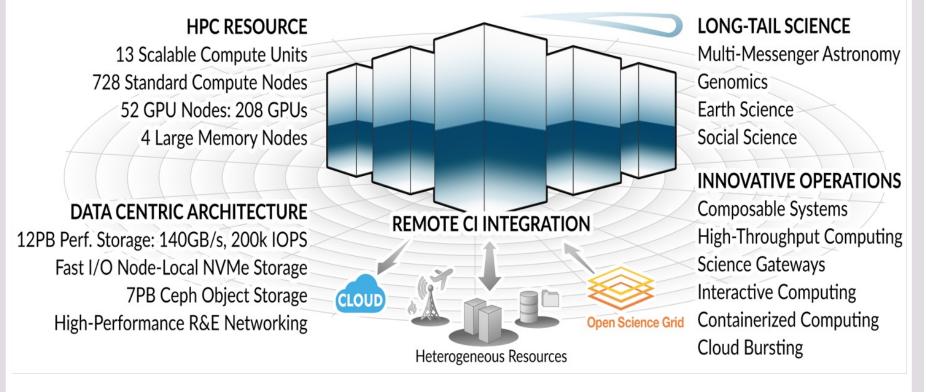
Carnegie Mellon University



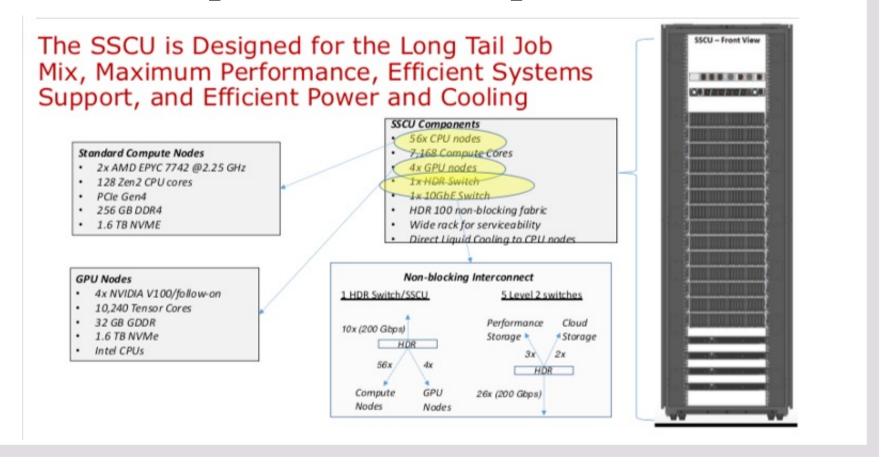


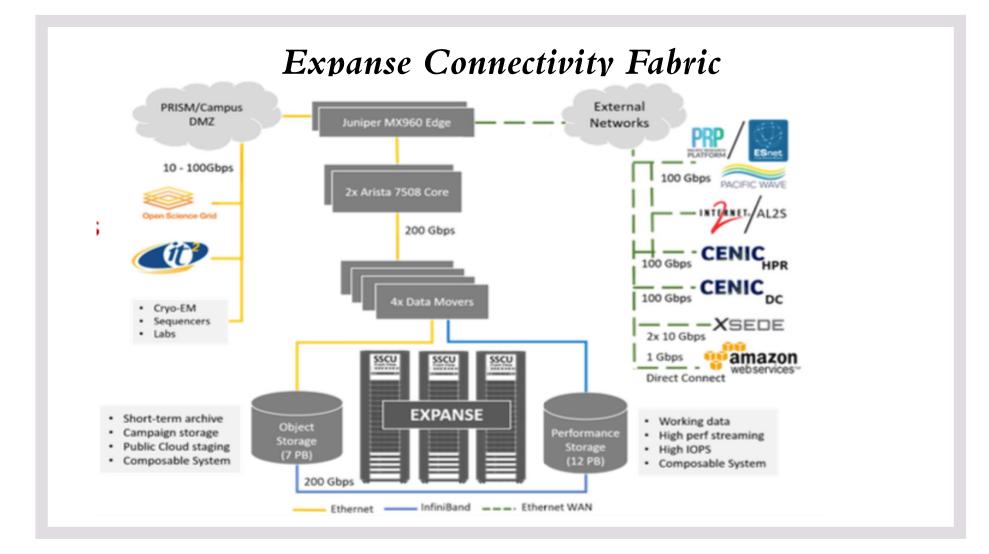


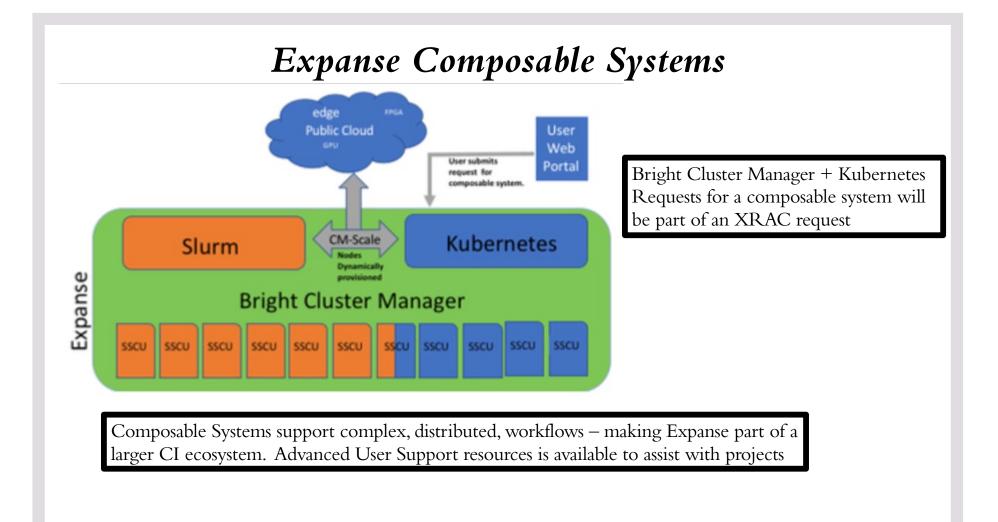
EXPANSE COMPUTING WITHOUT BOUNDARIES 5 PETAFLOP/S HPC and DATA RESOURCE



Expanse Scalable Compute Unit

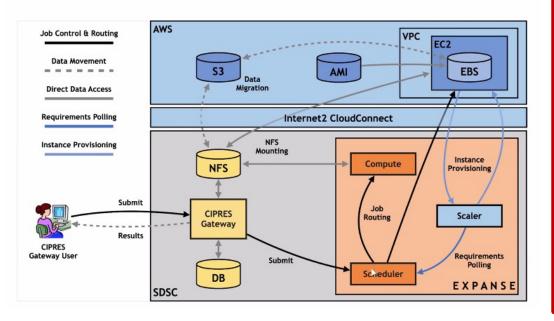




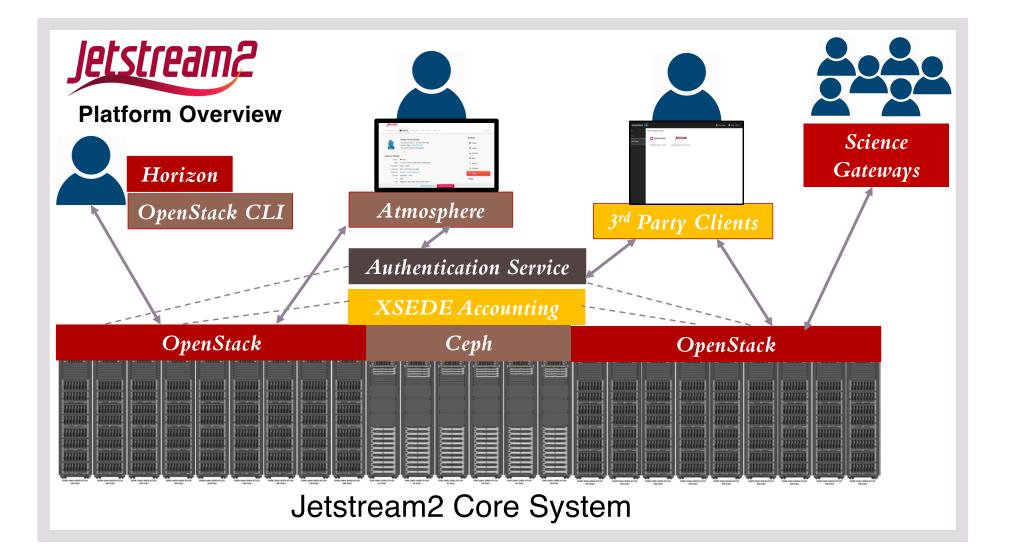


Expanse Cloud Bursting

Cloud Integration Technology



- Expanse supports integration with public clouds.
- Support for projects that share data, need access to novel technologies, and integrate cloud resources into workflows
- Users submit directly via Slurm, or as part of a composed system.
- Options for data movement: data in the cloud; remote mounting of file systems; cached filesystems (e.g., StashCache), and data transfer during the job.





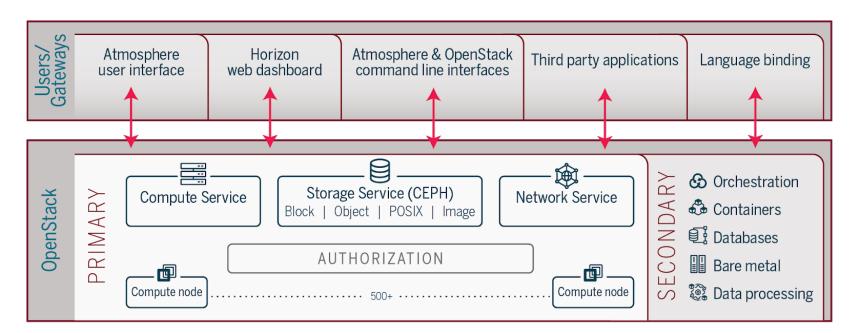
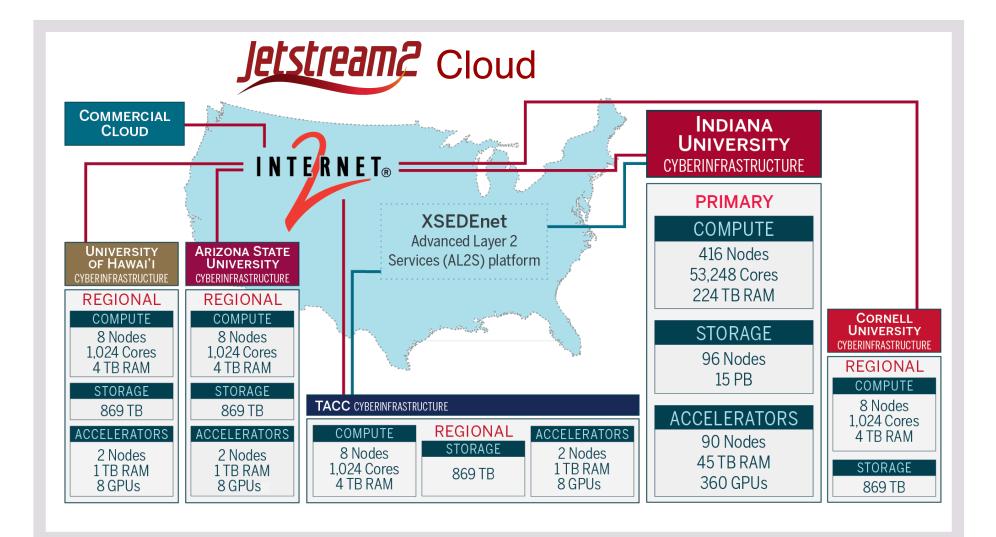


Figure 2: Conceptual and architectural diagram of the system environment



Jetstream? Capabilities

Jetstream@

Home > Project TG-CHE200061 > Create Instance

Jetstream2 IU - TG-CHE200061 (logged in as jfossota@xsede.org)

Create Instance

| Name * | jfosso-test-vm | | | | | |
|---|--|--|--|--|--|--|
| Image: Fe | Image: Featured-Ubuntu20 | | | | | |
| Flavor | | | | | | |
| General-p | ourpose | | | | | |
| • • • • • • • • • • • • • • • • • • • | Name m3.tiny m3.small m3.quad m3.medium m3.large m3.xl m3.2xl | CPUs 1 2 4 8 16 32 64 | RAM 3 GB 6 GB 15 GB 30 GB 60 GB 125 GB 250 GB | Root Disk 20 GB 20 GB 20 GB 60 GB 60 GB 60 GB 60 GB | Ephemeral Disk none none none none none none none | |
| Large-me | , | | | | | |
| X X | Name r3.large r3.xl | CPUs 64 128 | RAM 500 GB 1,000 GB | Root Disk 60 GB 60 GB | Ephemeral Disk none none | |
| GPU 🛈 | Name | CPUs | DAM | Boot Dick | Enhomoral Dick | |
| 0 0 X | Name g3.small g3.medium g3.large g3.xl | 4 8 16 32 | RAM 15 GB 30 GB 60 GB 125 GB | Root Disk 60 GB 60 GB 60 GB 60 GB | Ephemeral Disk none none none none | |

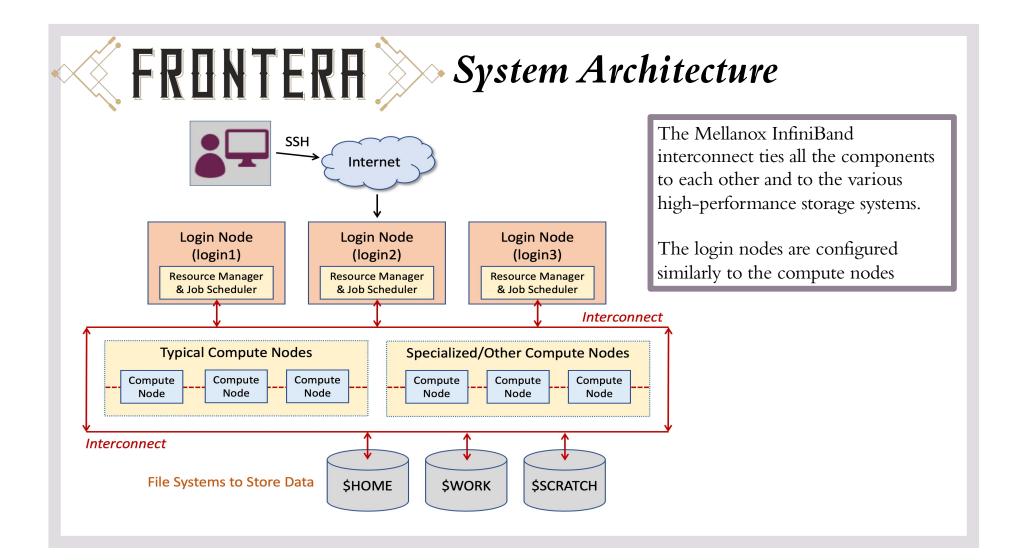
Enhancing laaS model of Jetstream:

- Improved orchestration support
- Elastic virtual clusters
- Federated JupyterHubs Commitment to >99% uptime
- Critical for science gateway hosting
- Hybrid-cloud support Revamped User Interface
- Unified instance management
- Multi-instance launch
- >57K cores of next-gen AMD EPYC processors
- >360 NVIDIA A100 GPUs will provide vGPUs via NVIDIA's MIG feature
- >18PB of storage (NVMe and disk hybrid)
- 100GbE Mellanox network

FRONTERR >>>>



| Object | Frontera |
|---------------------------------------|--|
| Compute Node Type | Intel Xeon Platinum 8280 ("Cascade Lake") |
| Total Nodes | 8,368 |
| Cores/Node | 56 (28 cores/socket with 2 sockets) |
| Hardware Threads/core | 1 |
| Clock Rate | 2.7 GHz Max Turbo: 4.0 GHz |
| Memory | 192 GB DDR4-2933 |
| Peak Memory Bandwidth ⁶ | 282 GB/s |
| L1 Cache | 32 KB per core |
| L2 Cache | 1 MB per core |
| L3 Cache | 38.5 MB per socket |
| Local Storage (/tmp) | 144 GB partition on 240 GB SSD |





The above graphic displays just a small subset of supported applications available on Frontera. *Singularity* is available through the *tacc-singularity* module on Frontera. It cannot be built on the system but can be developed locally, then upload to Frontera.

NSF/XSEDE →*ACCESS Systems* Efficient and Effective Use of Resources

Share your thoughts in the chat: state observed habits adopted by your users that have resulted in the wasteful usage of resources. What steps have you taken to reduce its occurrence?

The OSG Consortium

Open Science Pool (OSPool) provides researchers with *fair-share* access to computing and data capacity powered by *distributed high-throughput* computing (dHTC) technologies.

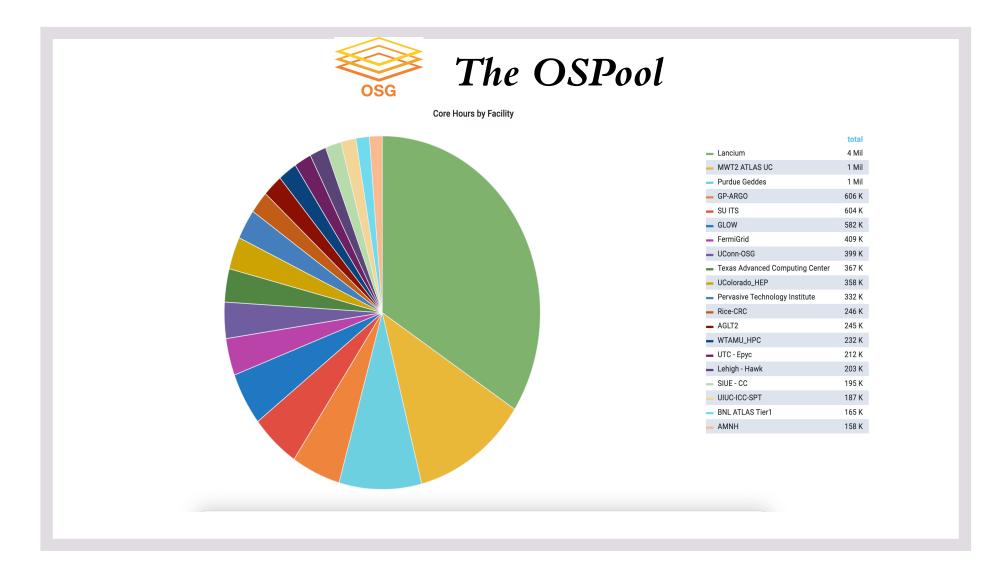


OSG All-Hands Meetings (AHM)

provides the consortium stakeholders and the broader dHTC community with a venue to *share ideas and exchange information*.

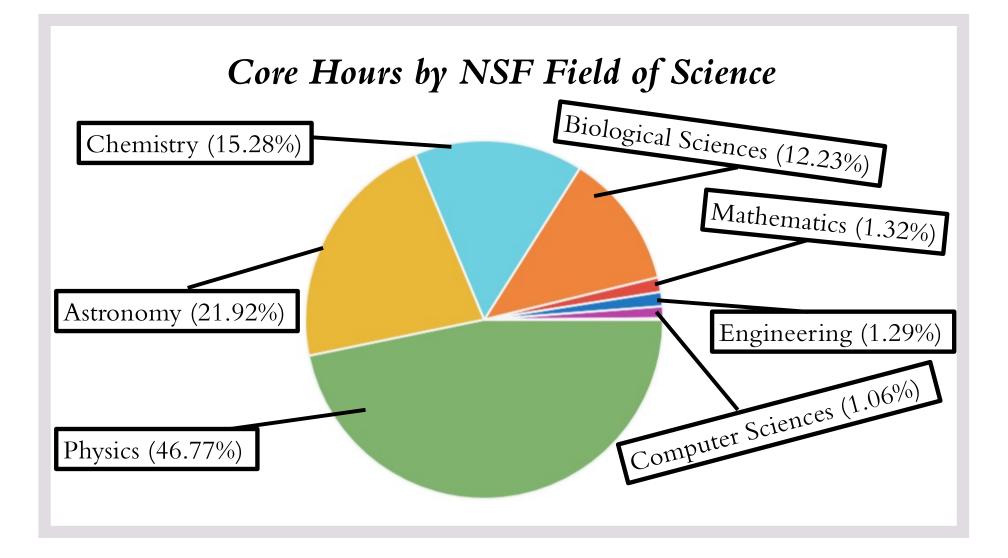
Open Science Data Federation (OSDF)

enables users and institutions to *share data files and storage capacity*, making them both accessible in dHTC environments such as the OSPool.





- Open to providers at all scales
 - from small colleges to large national labs
- Open to user communities at all scales
 - from individual students to large research communities
 - domain science specific and across many campuses
 - campus specific and across many domain sciences
- Open to any business model
 - sharing, allocations, purchasing
 - preemption is an essential part of operations



The OSG Consortium Compute Resource Consolidation

Share your thoughts in the chat: have you consolidated compute resources on your campus? What are the benefits of such an initiative?

$NSF/XSEDE \rightarrow ACCESS$ Systems

Systems Information

- □ *Allocated Resources*: general description of the resource and its recommended use.
- □ *Non-Allocated Resources*: information about other resources in the XSEDE ecosystem
- □ *Allocation Requests*: general information about resources and allocation requests.
- Link to information: https://portal.xsede.org/allocations/resource-info

DOE National Labs:

OLCF Summit Overview

The system includes:

- 4,608 nodes
- Dual-port Mellanox EDR InfiniBand network
- 250 PB IBM file system transferring data at 2.5 TB/s

Each node has:

- 2 IBM POWER9 processors
- 6 NVIDIA Tesla V100 GPUs
- 608 GB of fast memory (96 GB HBM2 + 512 GB DDR4)
- 1.6 TB of NV memory



System Performance:

- Peak of 200 Petaflops (FP64) for modeling & simulation
- Peak of 3.3 ExaOps (FP16) for data analytics and artificial intelligence

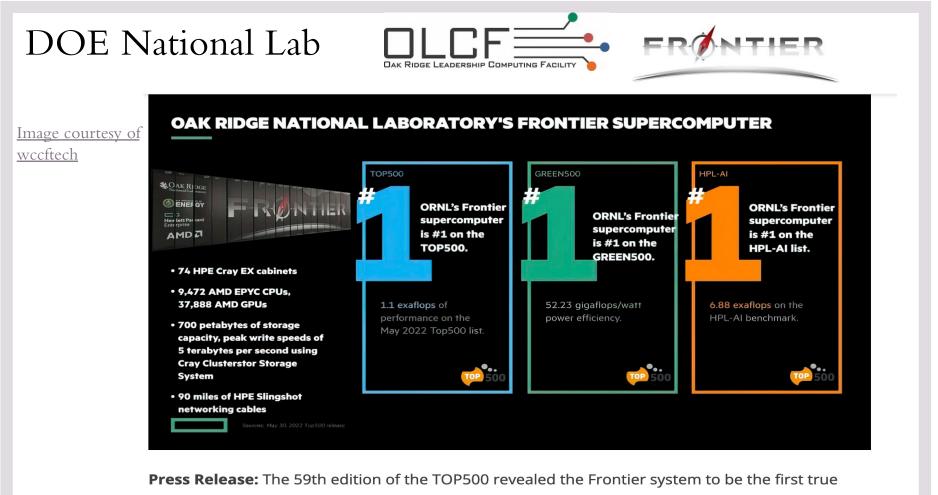
| | COMPUTING FACILITY |
|---|--------------------|
| 2 | |

| Feature | Summit |
|-----------------------|---------------------------------|
| Peak FLOPS | 200 PF |
| Max possible Power | 13 MW |
| Number of Nodes | 4,608 |
| Node performance | 42 TF |
| Memory per Node | 512 GB DDR4 + 96 GB HBM2 |
| NV Memory per Node | 1.6 TB |
| Total System Memory | 2.8 PB + 7.4 PB NVM |
| System Interconnect | Dual Port EDR-IB (25 GB/s) |
| Interconnect Topology | Non-blocking Fat Tree |
| Bi-Section Bandwidth | 115.2 TB/s |
| Processors om node | 2 IBM POWER9™ 6 NVIDIAVolta™ |
| File System | 250 PB, 2.5 TB/s, GPFS |



Summit

OLCF Summit Specs



exascale machine with an HPL score of 1.102 Exaflop/s.

| DOE National I | Lab |
|----------------|-----|
|----------------|-----|





| Feature | Frontier |
|----------------------|---|
| Peak FLOPS | > 1.5 EF |
| Cabinets | > 100 |
| Node | HPC and AI Optimized 3rd Gen AMD EPYC CPU Purpose Built AMD Instinct 250X GPUs |
| CPU-GPU Interconnect | AMD Infinity Fabric |
| System Interconnect | Multiple Slingshot NICs providing 100 GB/s network bandwidth. Slingshot network which provides adaptive routing, congestion management and quality of service. |
| Storage | 2-4x performance and capacity of Summit's I/O subsystem. Frontier will have near node storage like Summit. |

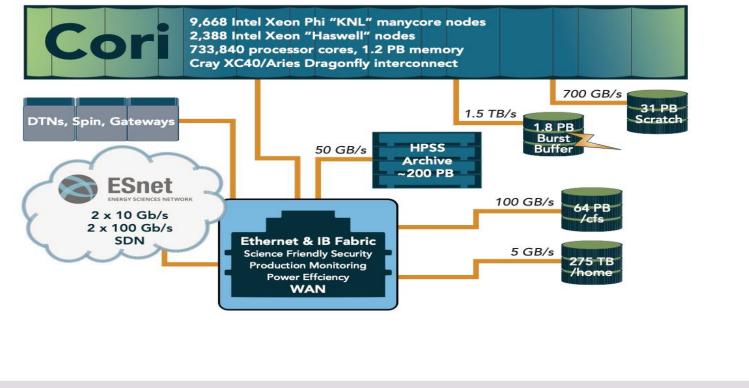


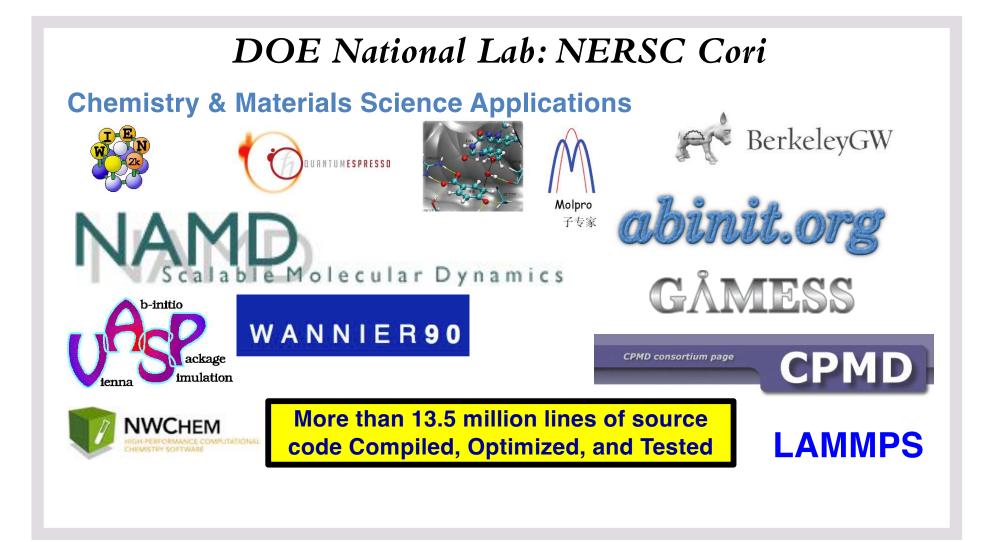
OLCF Frontier Specs

NB: Summit has 250 PB, 2.5 TB/s, GPFS

DOE National Lab: NERSC Cori

NERSC Systems

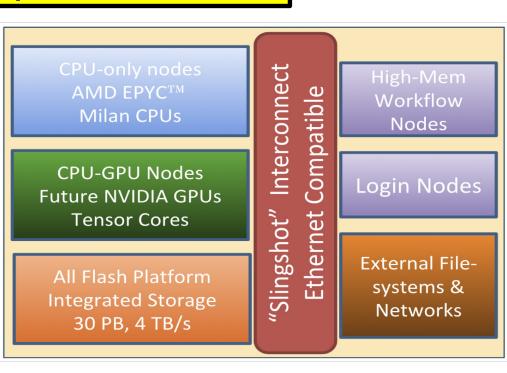




DOE National Lab: NERSC Perlmutter

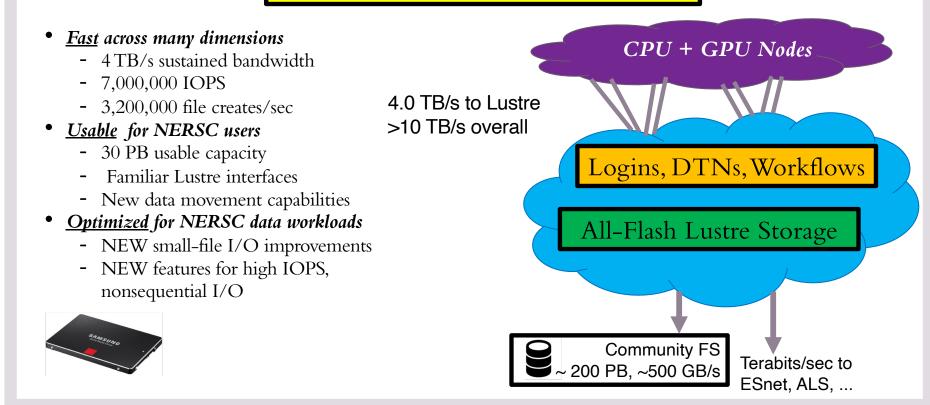
A System Optimized for Science

- GPU-accelerated and CPU-only nodes meet the needs of large-scale simulation and data analysis from experimental facilities
- Cray "Slingshot" High-performance, scalable, low-latency Ethernet compatible network
- Single-tier All-Flash Lustre based HPC file system, 6x Cori's bandwidth
- Dedicated login and high memory nodes to support complex workflows



DOE National Lab: NERSC Perlmutter

A System Optimized for Science



DOE National Lab

Share your thoughts in the chat: What are the similarities/differences between the DOE and XSEDE→ACCESS Systems?

DOE National Lab HPC Centers and Systems

- The National Renewable Energy Laboratory (NREL) <u>https://www.nrel.gov/hpc/</u>
- o Livermore Computing: HPC at LLNL <u>https://hpc.llnl.gov/</u>
- Los Alamos NL High Performance Computing <u>https://www.lanl.gov/org/ddste/aldsc/hpc/index.php</u>
- o Idaho NL HPC <u>https://hpc.inl.gov/SitePages/Home.aspx</u>
- Oak Ridge NL's Leadership Computing Facility <u>https://www.olcf.ornl.gov/</u>
- o Argonne NL's Leadership Computing Facility https://www.alcf.anl.gov/
- Sandia NL HPC https://hpc.sandia.gov/access/

Science Gateways

| Conn | Science Gateways Catalog ect people and resources to accelerate discovery by empowering the science gateway community |
|-------------------------------------|---|
| FIND A GATEWAY CATALOG | HELP/ABOUT |
| Total Entries: 632 | Sort by A-Z |
| FILTER BY: A Category: Gateway X | Arctos: Collaborative Collection Management Solution |
| GATEWAY (539) SGCI CLIENT (34) | GATEWAY Arctos is an ongoing effort to integrate access to specimen data, collection-management tools, and external resources on the internet. |
| USED IN CLASSROOM (45) | |
| PHYSICAL (264) 🗸 | Categories: Social, Anthropology, Archaeology, History |
| LIFE (257) 🗸 | Contact Info: arctos.database@gmail.com |
| SOCIAL (83) 🗸 | Tags: Arctos museum collection |
| APPLIED (157) 🗸 | |
| INTERDISCIPLINARY (157) 🗸 | |
| FORMAL (24) 🗸 | 20th Century Reanalysis Project 😐 |
| PHILOSOPHY (33) V | http://portal.nersc.gov/project/20C_Reanalysis/ |

Science Gateways simplify access to computing resources by hiding infrastructure complexities.

• Science Gateways provide higher level user interface for XSEDE resources that are tailored to specific scientific communities. (https://www.xsede.org/ecosystem/science-gateways/gateways-listing)

• A Science Gateway is a community developed set of tools, applications, and data that are integrated via a portal or a suite of applications, usually in a graphical user interface, that is further customized to meet the needs of a specific community

Science Gateways



Science Gateways Listing

XSEDE: https://www.xsede.org/web/site/ecosystem/science-gateways/gateways-listing

SGCI Catalog: https://catalog.sciencegateways.org/#/home

SGCI Catalog Summary

GATEWAY (264)

SGCI CLIENT (17)

USED IN CLASSROOM (28)

PHYSICAL (264) 🗸

LIFE (89) 🗸

SOCIAL (45) \vee

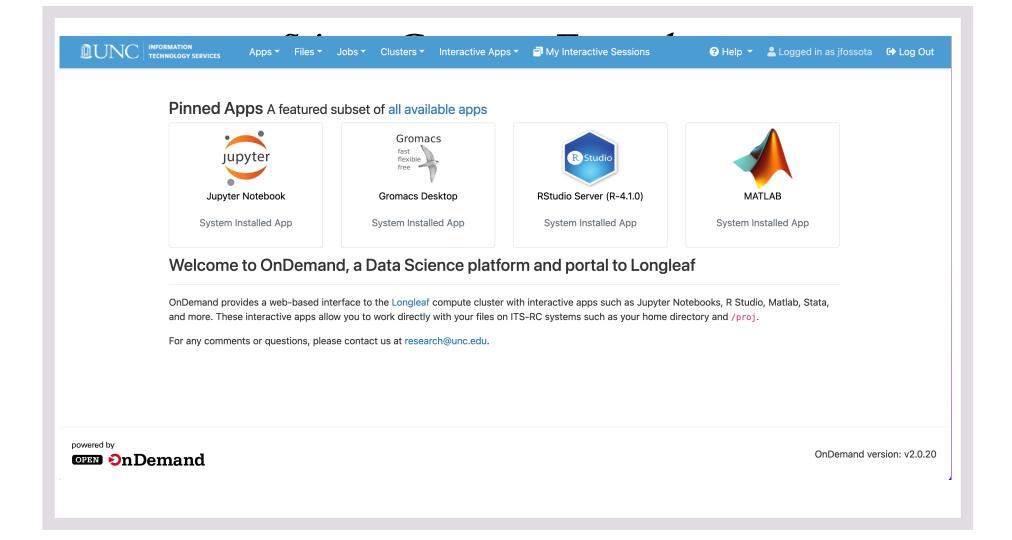
APPLIED (72) V

INTERDISCIPLINARY (73) \sim

FORMAL (18) 🗸

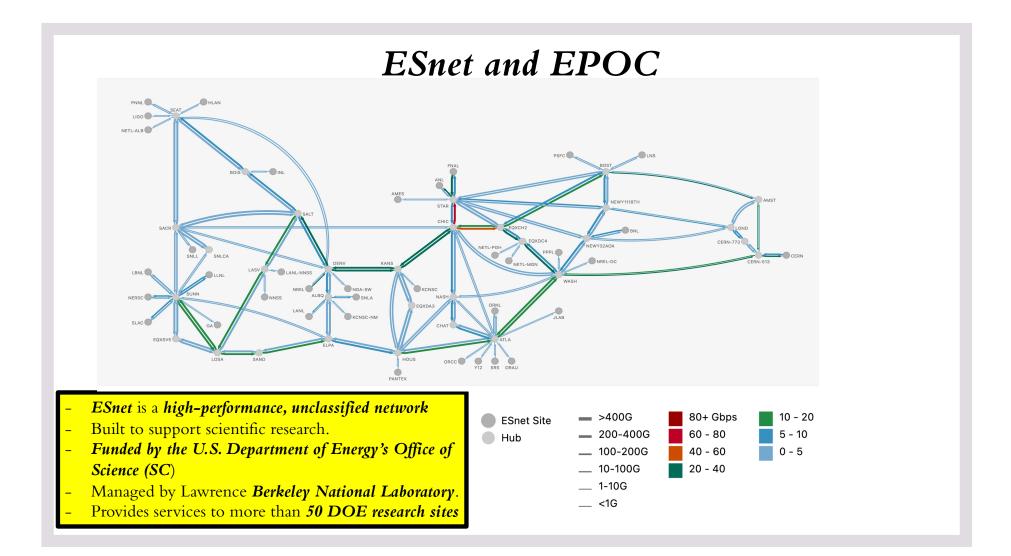
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|--|---|------------------------------------|---|----------------------------------|---|--------------|--|--|
| | Pinned Apps A featured subset of all availa | | Desktops ↓Longleaf Desktop Gromacs Desktop | | | | | |
| | Jupyter | Gromac fast flexible free | GUIs 3D Slicer | Studio | | | | |
| | Jupyter Notebook System Installed App | Gromacs De System Install | ton COMSOL IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII | erver (R-4.1.0) Installed App | MATLAB System Installed App | | | |
| | Welcome to OnDema | nd, a Data Scie | ◆ Freeview ○ GView | ortal to Longle | ortal to Longleaf | | | |
| OnDemand provides a web-based interface to the Longleaf and more. These interactive apps allow you to work directly For any comments or questions, please contact us at resear | | | MATLAB Mathematica Pymol RStudio Desktop SAS Spyder Stata | apps such as Jupyter N | otebooks, R Studio, Matlab, Stata, ectory and /proj. | | | |
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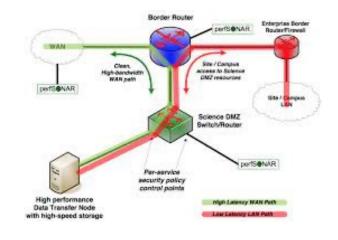
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| /datacommons | | | | □ Show | Owner/Mode | Show Dotfiles Filter: | |
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| | | | DMTCP-Tutorial | • • | - | 10/13/2021 3:34:02 PM | |
| | | • | dogwood | • • | - | 3/31/2020 7:14:47 AM | |
| | | • | LleafClusterJobs | • • | - | 7/24/2020 1:53:28 PM | |
| | | • | longleaf | • • | - | 3/31/2020 7:29:52 AM | |
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ESnet and EPOC

Esnet: Technical and Consulting Services

- The Science DMZ Architecture and Security
- Data Transfer Nodes
- perfSONAR
- Data transfer: Tools and Platforms
- Modern Research Data Portal.
- Network Requirements Gathering
- Collaboration
- Training Programs and Workshops
- Knowledge Base
- CI Engineering Lunch & Learn Series



https://www.es.net/science-engagement/technical-and-consulting-services/

ESnet and EPOC

EPOC: Six Main Activities

- <u>Roadside Assistance and consultation</u> via a coordinated Operations Center to resolve network performance problems with end-to-end data transfers reactively;
- <u>Application Deep Dive</u> to work more closely with application communities to understand full workflows for diverse research teams in order to evaluate bottlenecks and potential capacity issues
- <u>Network Analysis</u> enabled by the <u>NetSage</u> monitoring suite to proactively discover and resolve performance issues
- The <u>Data Mobility Exhibition</u> and associated work with our simplified portal to check transfer times against known "good" end points
- <u>Provision of managed data services</u> via support through the <u>IU GlobalNOC</u> and our <u>Regional Network Partners</u>
- Coordinated Training to ensure effective use of network tools and science support



NSF CC* Specific Resources

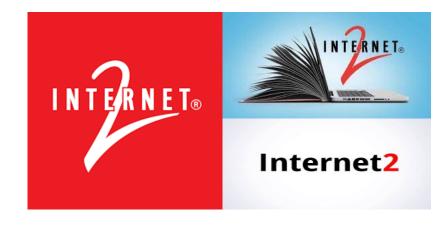
Including EPOC in a Proposal

https://epoc.global/proposal-collaborations/

Internet2

About Internet2

- Internet2 is a community:
 - Higher education and Research institutions
 - Government entities, corperations and cultural organizations
- Cyberinfrastructure provider:
 - secure high-speed network, cloud solutions,
 - research support, services tailored for research and education
- Through InCommon provides:
 - Security and privacy,
 - IAM tools for research and education,
 - single sign-on (SSO) for access to cloud local services and roaming wi-fi



Internet2

BY THE NUMBERS

ADVANCING SCHOLARSHIP

ACCELERATING DISCOVERY

320+ HIGHER EDUCATION MEMBERS

1000+ INCOMMON PARTICIPANTS

60 AFFILIATE & GOVERNMENT MEMBERS

46 REGIONAL & STATE NETWORKS 950+ EDUROAM SUBSCRIBERS

80,000+ COMMUNITY ANCHOR INSTITUTIONS

100+ COUNTRIES & RESEARCH NETWORKS CONNECTIONS

800G+ WAVELENGTHS OF NETWORK CAPABILITY 350+ NET+ SUBSCRIBERS

50+ INDUSTRY MEMBERS

750+ NET+ CLOUD CONTRACTS

32Tbps CAPACITY PER LINK

Internet2

| | | | | | Solutions | Services | News | Events | Contact | ٩ |
|-----------------------|---------------|---------------|-------------|--------------|-----------|----------|------|--------|---------|---|
| INTERNET _® | l Want To | Network | Security | Cloud | Commun | ity | | | | |
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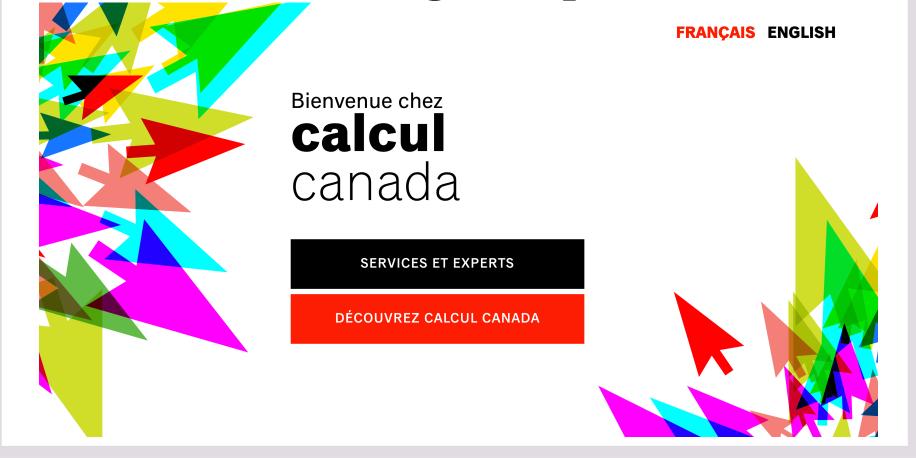
The Internet2 community works together to develop, vet, and provide services and software to meet the needs and requirements of research and education.

- *Cloud:* AWS, DocuSign, Duo Security, GCP, ServiceNow, Zoom, Splunk
- *InCommon:* COmanage, eduroam, InCommon Federation, Shibboleth

• Network:

Cloud Connect: Extend your data center to the cloud using the combination of your regional network and the Internet2 high-speed national

International Orgs: Compute Canada



International Orgs: Compute Canada

Research Portal

Account Management

National Services

Apply for an account

Account Renewals

Login to CCDB

Compute Canada CCV Submission Guide

User Roles to Access Resources and Services of the Compute **Canada Federation**

Clusters

Compute Canada Cloud

Storage

Data Movement (Globus)

Humanities and Social Sciences

Visualization

Accessing Resources

Resource Allocation Competitions

Rapid Access Service

Available Resources for RAC 2022

Technical Glossary

Acknowledging Compute Canada

Technical Support

Getting Help

Training

Documentation

International Orgs: GÉANT

Services

GÉANT develops and operates a range of connectivity, cloud, and identity services that ensure a safe and secure environment for researchers, educators, and students.

Community

The GÉANT Community Programme facilitates collaboration and knowledge sharing between NRENs, user organisations, R&E institutions, and the commercial sector.

Digital Inclusion



+50%

Bringing fibre connectivity to more of European research and education

GÉANT

GÉANT is the collaboration of European National Research and Education Networks (NRENs). Together we deliver an information ecosystem of infrastructure and services to advance research, education, and innovation on a global scale.

Network

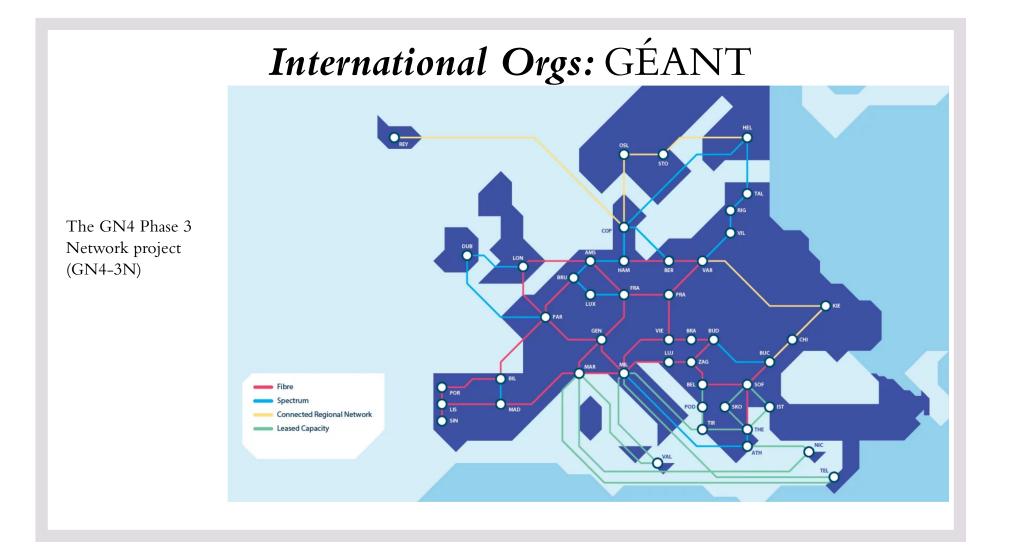
Europe's essential terabit network for research and education interconnects Europe's NRENs and links them to over 100 countries in every region of the world.

Data Growth



+30%

Average annual increase in network traffic over last five years



International Orgs:



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

<section-header>

HPC IN EUROPE PORTAL



The mission of PRACE is to enable high-impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society.

INDUSTRY & SMEs



TRAINING & SUPPORT



Cyberinfrastructure Tools

Share your thoughts in the chat: What is a cyberinfrastructure tool?

Cyberinfrastructure Tools OPEN ASK.CYBERINFRASTRUCTURE **OnDemand** Transfer your data. As a rule, tools can be D characterized as devices that help scientists do what they know they must do. fast METRICS ON DEMAND Ref:https://www.ncbi.nlm.nih.gov/books/NBK25460/ secure transfer reliable Jupyterhub **Prometheus** Pegasus Grafana Workflow Management

I Am Grateful For Your Attention. Thank You.