

# The CI Milieu: Systems, Service Providers, Technologies

Douglas M. Jennewein, Arizona State University,

Campus Champions Leadership Team

Virtual Residency

June 7, 2021



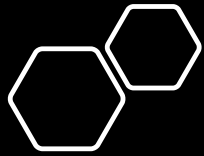
CAMPUS  
CHAMPIONS

*With support from:*



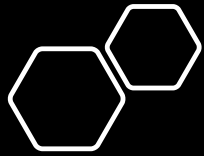
**XSEDE**

Extreme Science and Engineering  
Discovery Environment



This talk will  
(briefly) cover

- NSF/XSEDE Systems: Stampede2, Bridges2, Comet, Expanse, Jetstream(2), Frontera
- Open Science Grid (OSG)
- Science Gateways
- NERSC: Cori and Perlmutter
- ESnet and EPOC
- Internet2
- International Orgs: GEANT, Compute Canada, PRACE
- Tools: Globus, XDMod, Spack, Open OnDemand, ask.ci



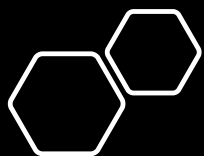
But first...

This talk will NOT cover:

- NSF Comet, Voyager, Ookami, Neocortex, Darwin, Delta, KYRIC, Anvil, CloudLab, Chameleon, and CloudBank
- NIH resources such as BioWulf
- Commercial Cloud
- Regional Networks and The Quilt

Only because of:

1. Time
2. Availability



# About XSEDE allocations

The screenshot shows the XSEDE website interface. At the top, there is a navigation bar with links for 'User Portal', 'Web Site', and 'Go to'. The XSEDE logo and tagline 'Extreme Science and Engineering Discovery Environment' are prominently displayed. A search bar is located in the top right corner. Below the navigation bar, the page title 'Campus Champions Allocations' is centered. The main content area is divided into two columns. The left column contains an 'Introduction' section, an 'IMPORTANT' notice, and a 'Starting an allocation request' section with a list of steps. The right column features a 'Campus Champions' sidebar with a 'Welcome' section and a list of links: 'Overview', 'How does it work?', 'For New Champions', 'Champion Allocations', 'Introductory Tutorials', and 'Current Champions'.

User Portal Web Site Go to

XSEDE  
Extreme Science and Engineering  
Discovery Environment

Search XSEDE...

CAMPUS CHAMPIONS HOME XSEDE USER PORTAL

## Campus Champions Allocations

### Introduction

Campus Champions are entitled to login access to computational facilities and the XSEDE User Portal just as any user of XSEDE. In order to gain such access, each champion must apply for a Champion startup allocation using the instructions below.

**IMPORTANT:** Please note that the purpose of this allocation is to allow you to become familiar with the resources, and to allow your users to gain quick access to perform the minimal tests and benchmarks needed to determine which resources they need for their research. Once this has been determined, your users should **immediately** request their own Startup Allocation. They can use this to start their research and get further benchmarks while they prepare a full Research Allocation proposal to be reviewed by the XSEDE Resource Allocation Committee (XRAC). Your users should **not** run production research calculations on your Champion Startup Allocation! Fortunately, the process for getting a Startup Allocation is quite easy (see below for Champion Startup Allocation).

### Starting an allocation request

Go to: [The XSEDE User Portal](#)

If you do not have an XSEDE Portal account, click on "Create Account" and follow the directions there.

Now log in to the XSEDE User portal and do the following:

- Click on the "Allocations" tab.
- Click on the "Submit/Review Request" link
- Select: "Campus Champions" under the Opportunities

For step by step instructions on how to use the XRAS system please read the [Getting Started Guide](#).

### Campus Champions

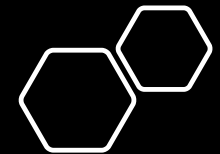
Welcome

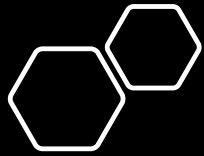
- Overview
- How does it work?
- For New Champions
- Champion Allocations
- Introductory Tutorials
- Current Champions



# Stampede2

The Flagship Supercomputer of XSEDE





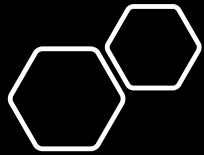
# Stampede2: Everything's Bigger in Texas

Brought online in 2017

Largest XSEDE system (and largest university-based system at the time)

18 petaflops of peak performance

Successfully launched 350,000MPI tasks in a single job

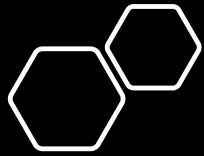


# Stampede2: Everything's Bigger in Texas

4,200 Intel Knights Landing nodes, each with 68 cores, 96GB of DDR RAM, and 16GB of high speed MCDRAM

1,736 Intel Xeon Skylake nodes, each with 48 cores and 192GB of RAM

100 Gb/sec Intel Omni-Path network with a fat tree topology employing six core switches



# Stampede2: Everything's Bigger in Texas

Stampede2 is intended primarily for **parallel applications scalable to tens of thousands of cores**, as well as general purpose and throughput computing.



Case in point: Successfully launched 350,000MPI tasks in a single job





Converged HPC, AI & Big Data for Rapidly-Evolving Research  
A PSC RESOURCE



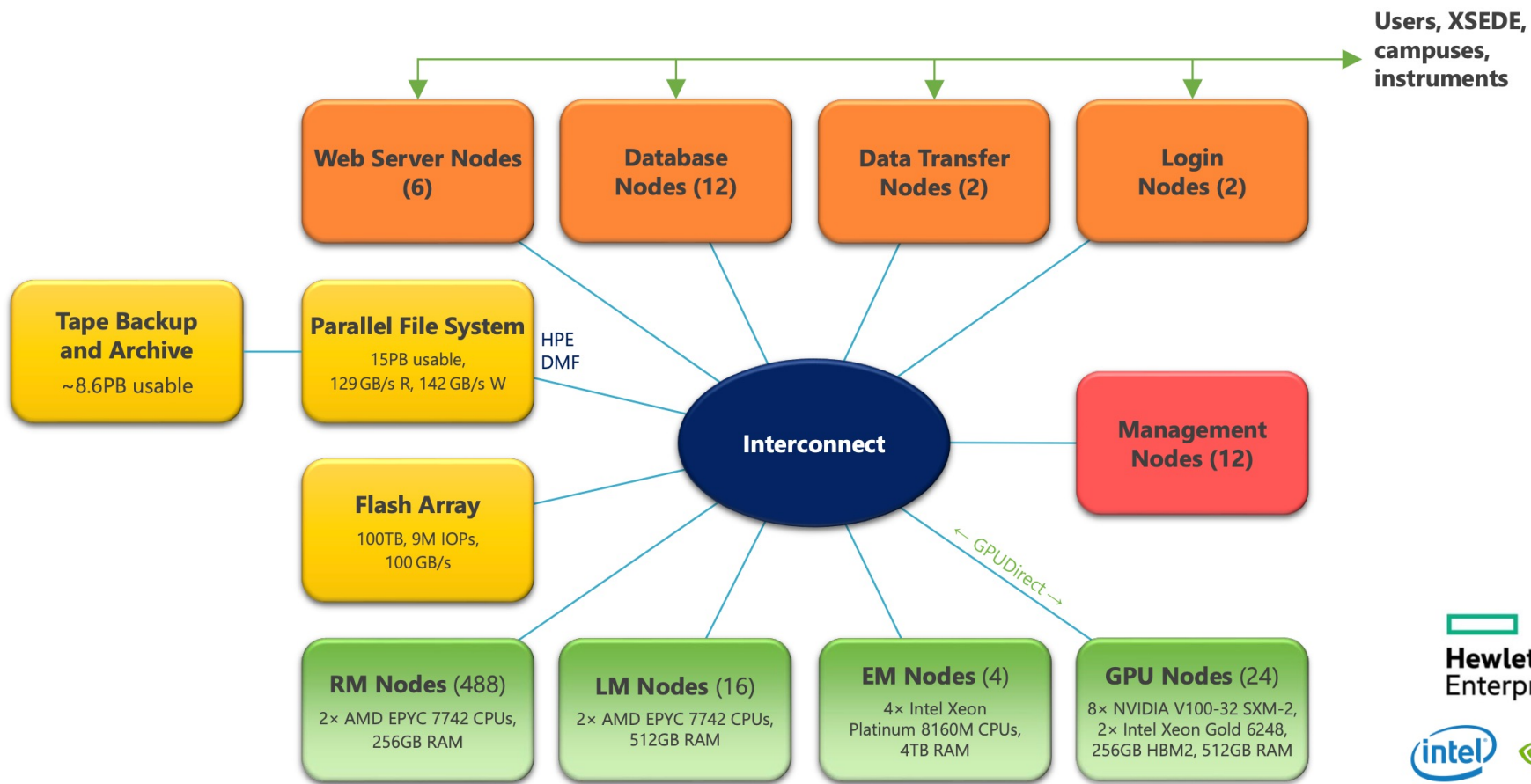
**Carnegie Mellon University**



University of Pittsburgh

Empowering New Research  
Communities, Bringing Together HPC,  
AI, and Big Data





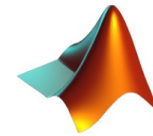
Carnegie Mellon University

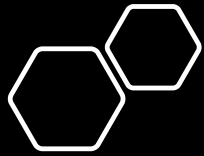


University of Pittsburgh



- Interactivity
- Popular languages and frameworks: Python, Anaconda, R, MATLAB, Java, Spark, Hadoop
- AI frameworks: TensorFlow, Caffe2, PyTorch, etc.
- Containers and virtual machines (VMs)
- Databases
- Gateways and distributed (web) services
- Large collection of applications and libraries





# Memory Intensive Applications

de novo and metagenome sequence assembly

graph analytics

large in-memory databases

machine learning applications

large-memory applications written in threaded languages

bioinformatics

causal analysis

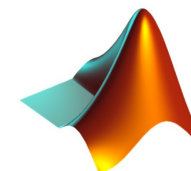
machine learning

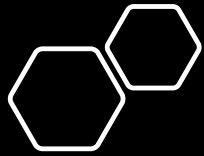
graph analytics



# Interactivity

- Interactivity is the feature **most frequently requested** by nontraditional HPC communities.
- Interactivity provides **immediate feedback** for doing exploratory data analytics and testing hypotheses.
- Bridges2 offers interactivity through a combination of **shared, dedicated, and persistent resources** to maximize availability while accommodating diverse needs.
- Provides languages and environments that **users already know**: High-Productivity Programming





Shared,  
dedicated,  
and  
persistent

Dedicated database nodes power persistent relational and NoSQL databases

Dedicated web server nodes

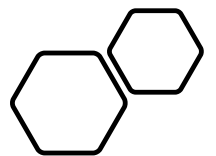
OpenStack, KVM, Singularity

Persistent community data collections: e.g. BLAST, ImageNet

# EXPANSE

COMPUTING WITHOUT BOUNDARIES

EXPANSE



# EXPANSE

COMPUTING WITHOUT BOUNDARIES  
5 PETAFLOP/S HPC and DATA RESOURCE

## HPC RESOURCE

- 13 Scalable Compute Units
- 728 Standard Compute Nodes
- 52 GPU Nodes: 208 GPUs
- 4 Large Memory Nodes

## LONG-TAIL SCIENCE

- Multi-Messenger Astronomy
- Genomics
- Earth Science
- Social Science

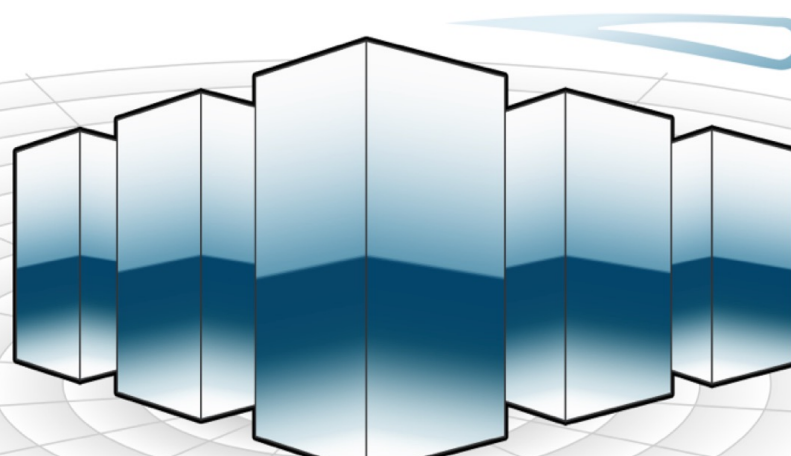
## DATA CENTRIC ARCHITECTURE

- 12PB Perf. Storage: 140GB/s, 200k IOPS
- Fast I/O Node-Local NVMe Storage
- 7PB Ceph Object Storage
- High-Performance R&E Networking

## REMOTE CI INTEGRATION

## INNOVATIVE OPERATIONS

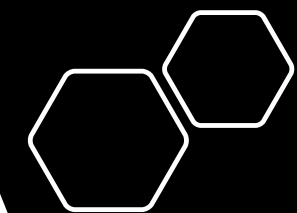
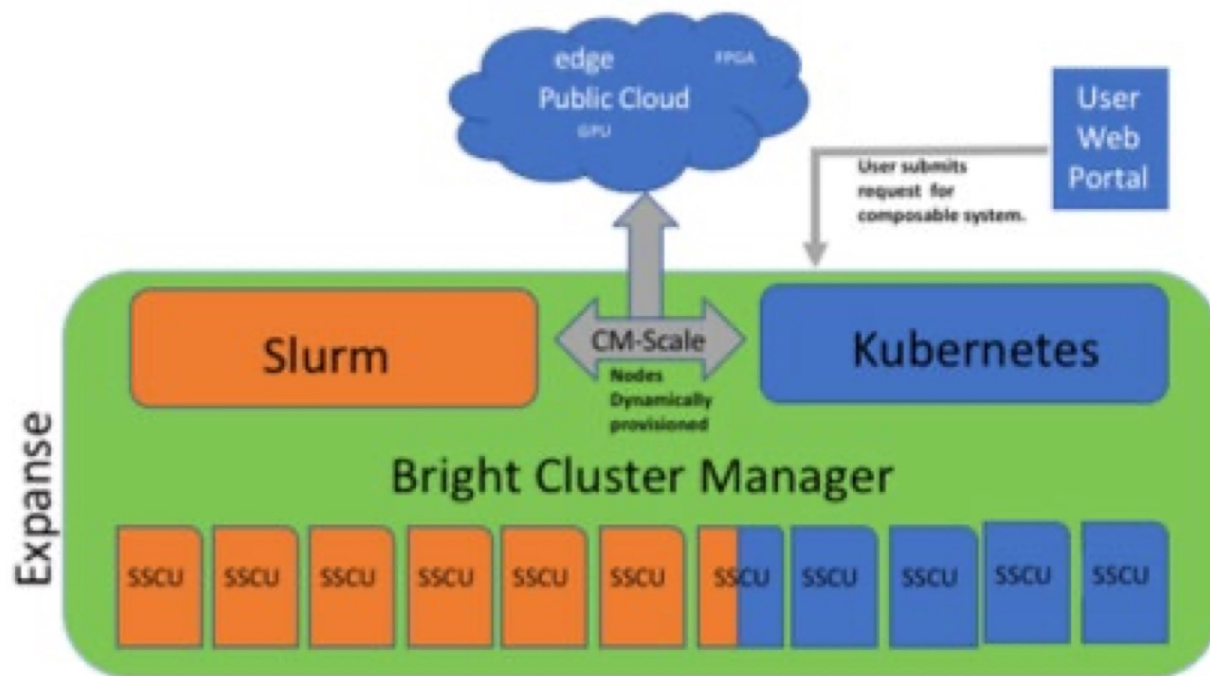
- Composable Systems
- High-Throughput Computing
- Science Gateways
- Interactive Computing
- Containerized Computing
- Cloud Bursting



Heterogeneous Resources

Open Science Grid





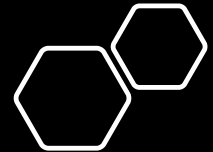
COMPOSABLE

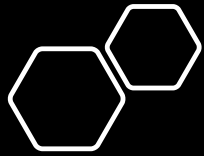


**PERVASIVE  
TECHNOLOGY INSTITUTE**

***Jetstream***

A NATIONAL SCIENCE AND  
ENGINEERING CLOUD






All cloud  
all the time


For the researcher needing a handful of cores on demand as well as for software creators and researchers needing to create their own **customized virtual machine** environments. Jetstream is accessible **ONLY** via web interface.

### Getting Started




**Launch New Instance**

Browse Atmosphere's list of available images and select one to launch a new instance.



**Browse Help Resources**

View a video tutorial, read the how-to guides, or email the Atmosphere support team.



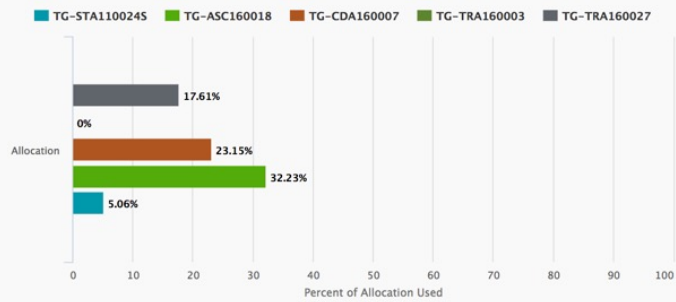
**Change Your Settings**

Modify your account settings, view your resource quota, or request more resources.

### Resources Used

[Need more?](#)

#### Allocation Source



#### 10 Instances

active shutoff

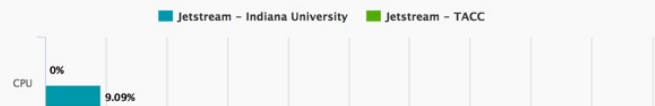


#### 4 Volumes

available



#### Provider Resources









## Image Search

Search across image name, tag or description

Showing 57 of 57 images

### Featured Images

-  **Centos 7 (7.2) Development GUI**  
Jan 13th 17 03:21 by [jfisher](#)  
Imported Application - Centos 7 (7.2) Development GUI  
[CentOS](#) [development](#) [Featured](#) [gui](#) [IRODS](#)
-  **BioLinux 8**  
Jan 2nd 17 03:34 by [jfisher](#)  
Based on Ubuntu 14.04.3 -Trusty Tahr - server - cloudimg  
--\*\*REQUIRES m1.small instance ...  
[bioinformatics](#) [desktop](#) [Featured](#) [gui](#) [m1\\_small](#) [Ubuntu](#) [x2go](#)
-  **Ubuntu 14.04.3 Development GUI**  
Jan 2nd 17 01:24 by [jfisher](#)  
Based on Ubuntu 14.04.3 Development Patched up to date as of 12/15/16 Base Ubuntu 14.04.3 ...  
[desktop](#) [development](#) [Featured](#) [gui](#) [IRODS](#) [Ubuntu](#) [vnc](#)
-  **Intel Development (CentOS 7)**  
Nov 30th 16 12:04 by [jfisher](#)  
**Intel compilers and development environment**  
\*REQUIRES a m1.small or larger VM to la ...  
[CentOS](#) [desktop](#) [development](#) [Featured](#) [gui](#) [Intel](#) [m1\\_small](#) [vnc](#)
-  **R with Intel compilers (CentOS ...)**  
Nov 30th 16 11:53 by [jfisher](#)  
R with Intel compilers built on CentOS 7 (7.3)  
\*\* Requires m1.small or greater sized VM \* ...  
[CentOS](#) [desktop](#) [development](#) [Featured](#) [gui](#) [Intel](#) [m1\\_small](#) [vnc](#)
-  **Galaxy Standalone**  
Nov 15th 16 04:49 by [admin](#)  
Galaxy 16.01 Standalone - based on Ubuntu 14.04.4 LTS  
This is a standalone Galaxy server ...  
[community-contributed](#) [Featured](#) [m1\\_large](#) [Ubuntu](#)

Jetstream Dashboard | Projects | Images | Help | Admin | jfischer

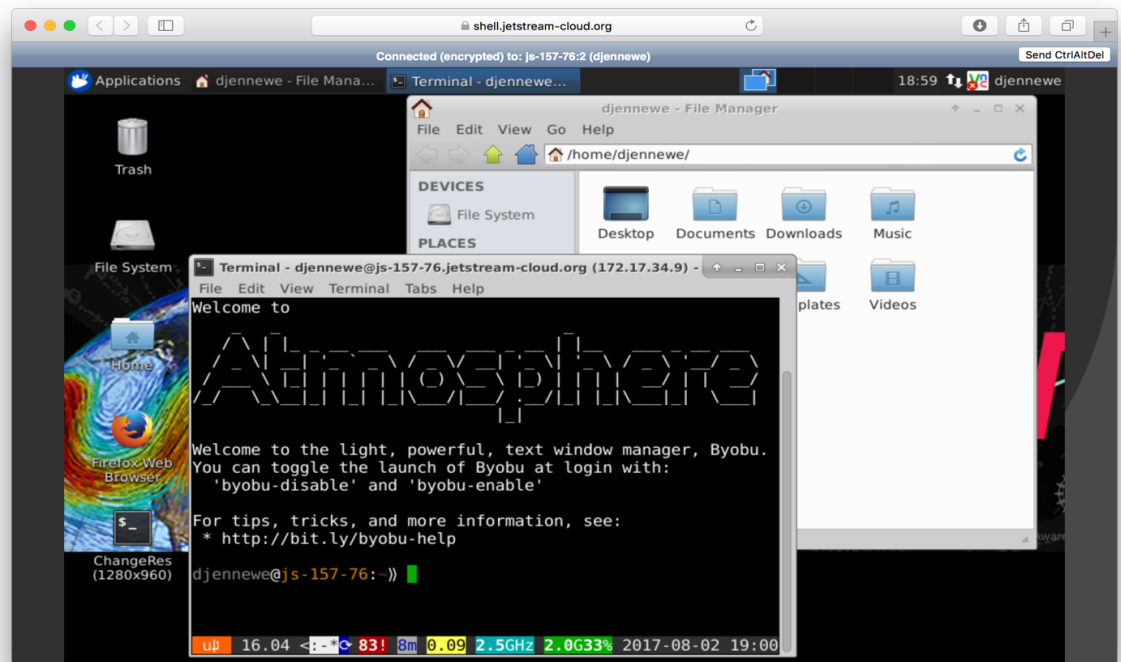
### Launch an Instance / Basic Options

Basic Info	Resources
<b>Instance Name</b> R with Intel compilers (CentOS 7)	<b>Allocation Source</b> TG-CIE170025
<b>Base Image Version</b> 1.14	<b>Provider</b> Jetstream - Indiana University
<b>Project</b> JLF Test	<b>Instance Size</b> m1.tiny (CPU: 1, Mem: 2 GB, Disk: 8 GB)
<b>Allocation Used</b> 0% of 140000 SUs from TG-CIE170025	
<b>Resources Instance will Use</b> A total 14 of 132 allotted CPUs	
A total 38 of 360 allotted GBs of Memory	

← Back   [Advanced Options](#)   CANCEL   LAUNCH INSTANCE

Jetstream Homepage - Jetstream Partners - Citing Jetstream - Jetstream is supported by NSF ACI-1445604   [FEEDBACK & SUPPORT](#)

Real  
screenshot  
from real  
iPad



## Jetstream2 Capabilities

Enhancing IaaS 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

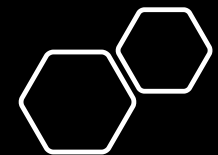
*Jetstream2*



Feb 12, 2019 – Jet stream region called "Jet N6"  
NASA/JPL-Caltech/SwRI/MSSS/Kevin M. Gill

- >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

# Jetstream2 coming soon!



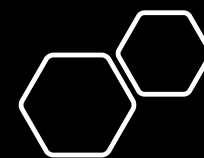


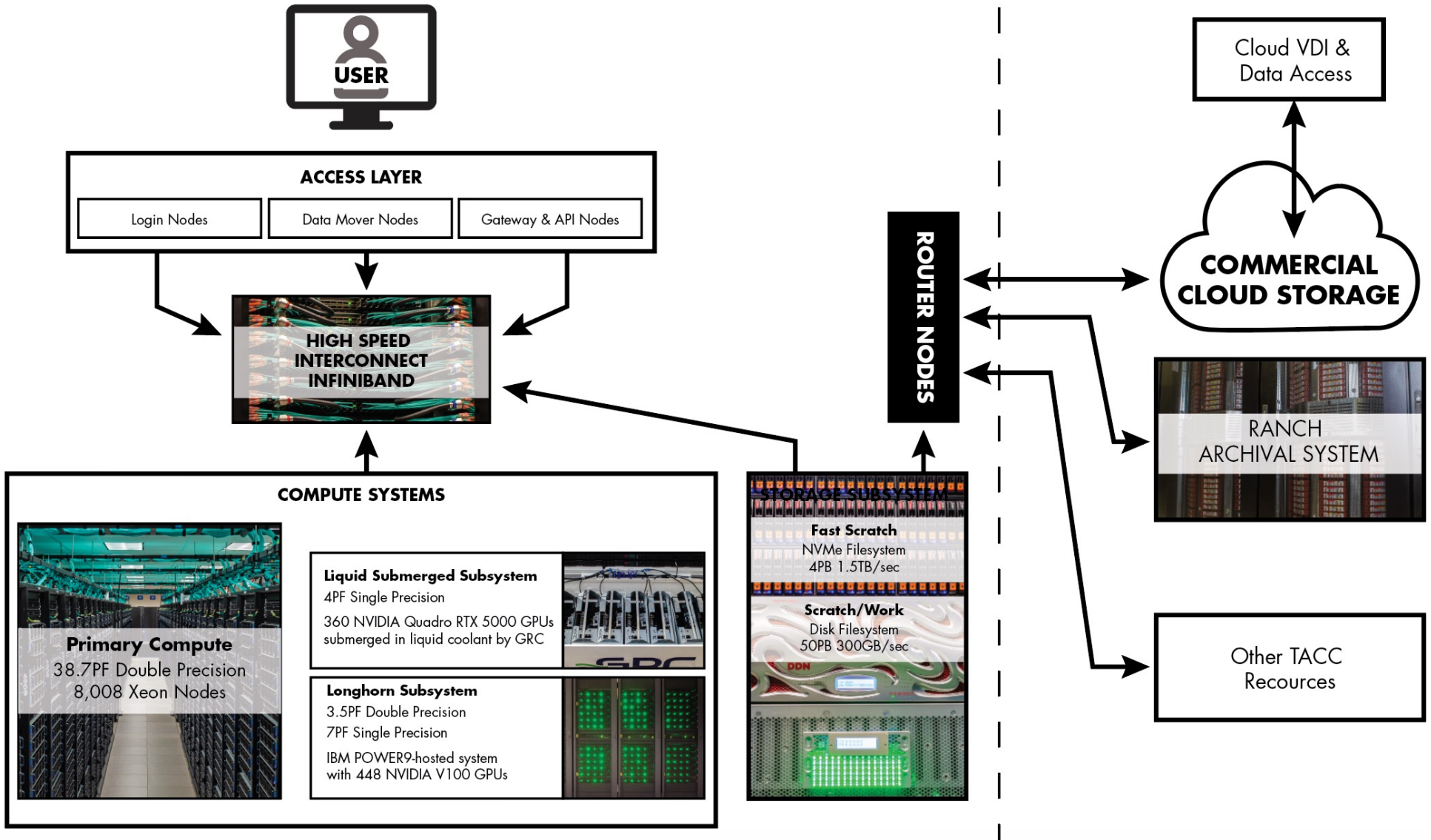
A banner graphic for the Frontiera program. On the left, a portion of Earth is visible in space. The word "FRONTERA" is written in a large, white, blocky font with a yellow outline. To the right of the text, a stylized figure in a white and orange outfit is shown in a dynamic, forward-leaning pose. The background is a dark blue space with a network of glowing orange lines and nodes, resembling a circuit board or data network. The right side of the banner transitions into a solid orange-red color.

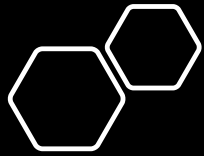
# FRONTERA

TACC | NSF | TEXAS

FRONTERA – LEADERSHIP CLASS  
COMPUTING



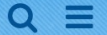




ALLOCATIONS  
ARE  
DIFFERENT



National Science Foundation  
WHERE DISCOVERIES BEGIN



[Email](#) [Print](#) [Share](#)

NSF 20-018

## Dear Colleague Letter: Frontera Leadership-Class Computing Allocations

November 6, 2019

Dear Colleagues:

Powerful new computing and data analytics capabilities are enabling novel discoveries and advances in knowledge not otherwise possible, which are in turn contributing to enhanced economic competitiveness and increased national security. Researchers in many areas of science and engineering (S&E) are pursuing innovative computational approaches to advance our understanding of the natural world, for example, by substantially increasing the resolution of computer simulations and expanding the use of predictive data-driven models derived from large experimental data sets often from disparate sources. As a result, advanced computational

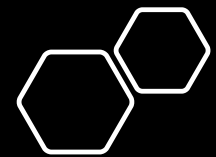


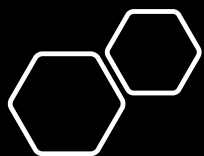
U.S. DEPARTMENT OF  
**ENERGY**

Office of Science



THE NATIONAL ENERGY RESEARCH  
SCIENTIFIC COMPUTING CENTER

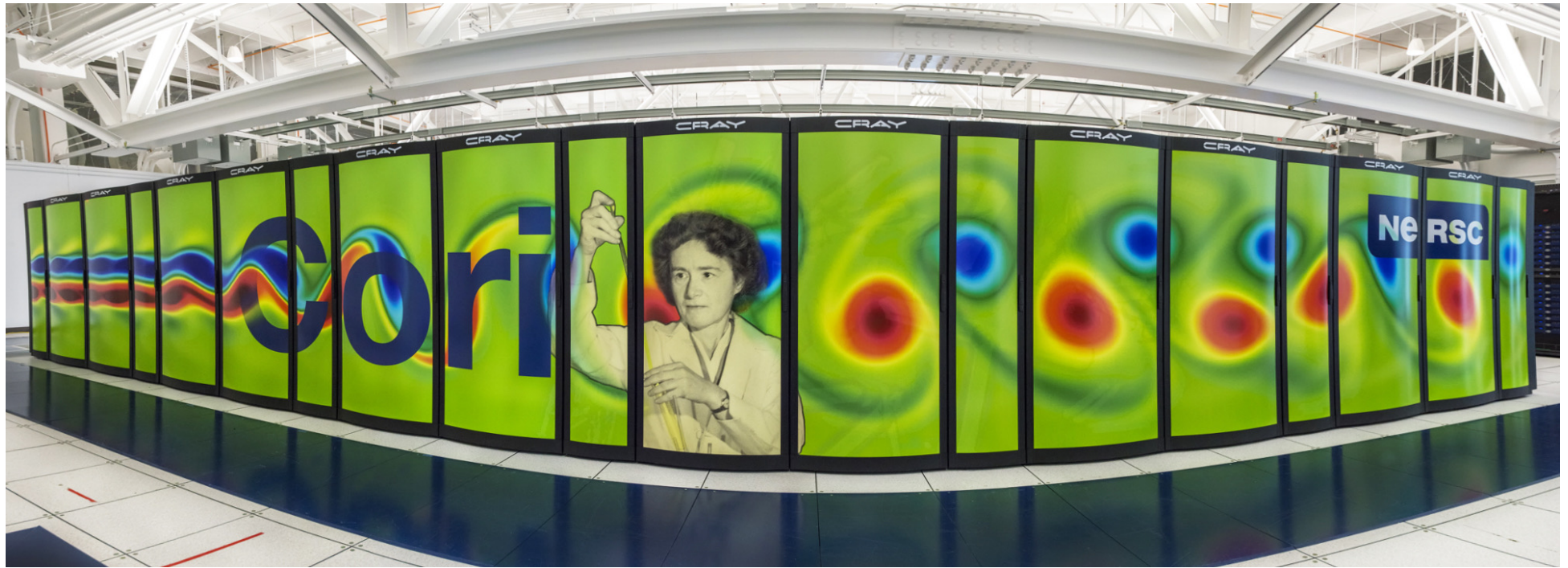




The text "NERSC" is written in a bold, white, sans-serif font. It is centered within a dark blue rectangular area that features a bright blue starburst or lens flare effect emanating from behind the letters.

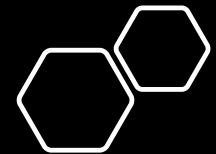
The National Energy Research Scientific Computing Center (NERSC) is the primary scientific computing facility for the [Office of Science](#) in the [U.S. Department of Energy](#).

All research projects that are funded by the DOE Office of Science and require high performance computing support are eligible to apply to use NERSC resources. **Projects that are not funded by the DOE Office of Science, but that conduct research that supports the Office of Science mission [may also apply](#).**



## System Overview

System Partition	# of cabinets	# of nodes	Aggregate Theoretical Peak	Aggregate Memory
Login	-	20	-	-
Haswell	14	2,388	2.81 PFlops	298.5 TB
KNL	54	9,688	29.5 PFlops	1.09 PB
Large Memory	-	20	30.7 TFlops	40 TB

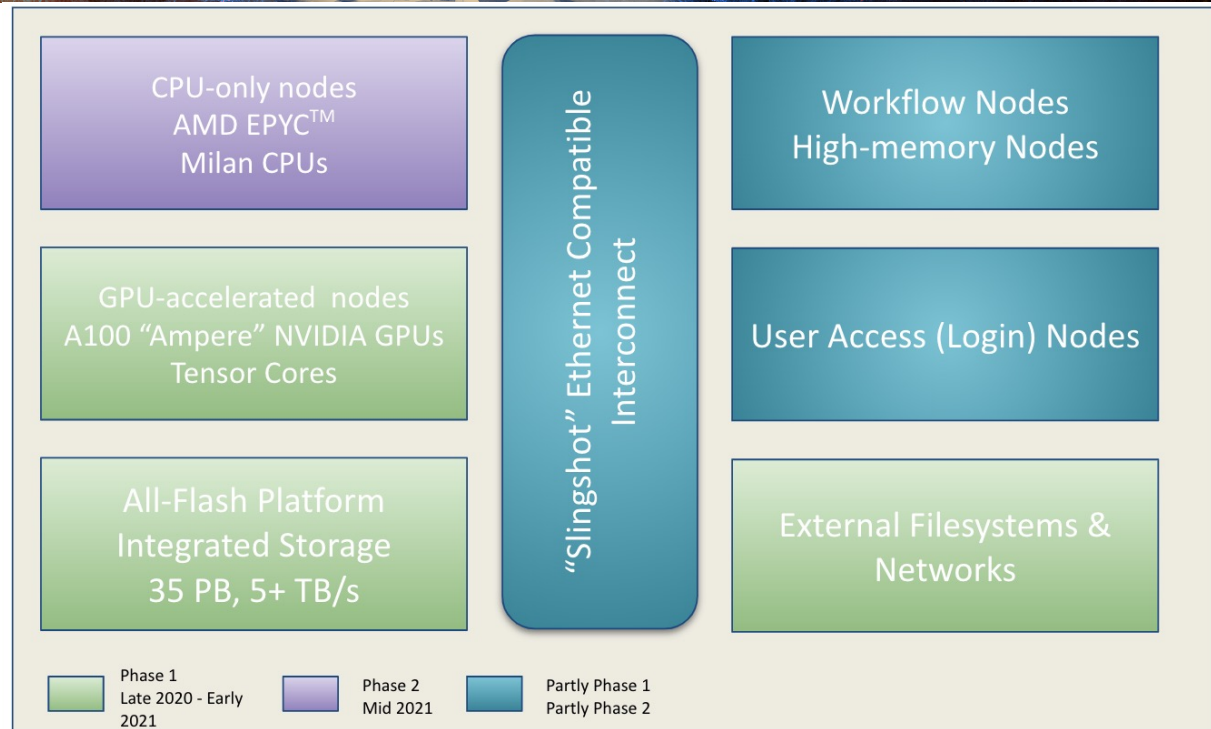


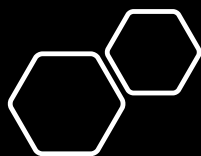
NERSC

# Perlmutter



COMING  
SOON





# ALLOCATIONS ARE DIFFERENT

The screenshot shows the NERSC website interface. At the top left is the NERSC logo with the tagline "Powering Scientific Discovery Since 1974". To the right is a search bar and a "My NERSC" link. Below the header is a navigation menu with items: HOME, ABOUT, COVID-19 RESEARCH, SCIENCE, SYSTEMS, FOR USERS (highlighted), NEWS, R & D, EVENTS, and LIVE STATUS. The breadcrumb trail reads: Home » For Users » Accounts & Allocations » Allocations » Allocation Request Form (ERCAP). The main heading is "THE NERSC ALLOCATION REQUEST FORM (ERCAP)". The text explains that requests are submitted annually via a web form known as the ERCAP (Energy Research Computing Allocations Process) Request Form, which is available year-round. It also suggests reading "Applying for your First NERSC Allocation" for new users. A section titled "Preparing an ERCAP Request" describes the procedures for starting a request, renewing a project, or editing an in-progress request. A numbered list provides the first step: pointing the browser to <https://ercap.nersc.gov> and logging in. A table of contents on the right lists seven steps: 1. Preparing an ERCAP Request, 2. Answering ERCAP Request Questions, 3. Submitting your request, 4. Printing and Saving to Disk, 5. Advice for Answering Long Text Questions, 6. ERCAP error messages, and 7. Deleting a request. A left-hand menu under "FOR USERS" lists various options, with "Allocation Request Form (ERCAP)" highlighted in green.

**NERSC** Powering Scientific Discovery Since 1974

Logi My NERSC | Share search... >>

HOME ABOUT COVID-19 RESEARCH SCIENCE SYSTEMS **FOR USERS** NEWS R & D EVENTS LIVE STATUS

Home » For Users » Accounts & Allocations » Allocations » Allocation Request Form (ERCAP)

## THE NERSC ALLOCATION REQUEST FORM (ERCAP)

Requests to use NERSC resources are submitted annually via a web form known as the **ERCAP** (Energy Research Computing Allocations Process) **Request Form**. The form is available year-round.

If you are new to NERSC read [Applying for your First NERSC Allocation](#).

### Preparing an ERCAP Request

The procedures for starting an ERCAP request for a new project, renewing a project and editing an in-progress request that you previously saved are described below.

1. Point your browser to <https://ercap.nersc.gov> and login. If you don't see the page show below, click on "ERCAP Request" from the list of items in the left-hand menu and chose the sub-menu item that applies. (If you don't see the left-hand menu, you may need to click on a little icon with an arrow within a circle at the bottom left of the screen.)

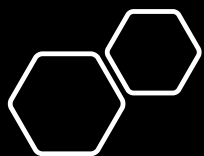
#### TABLE OF CONTENTS

1. Preparing an ERCAP Request
2. Answering ERCAP Request Questions
3. Submitting your request
4. Printing and Saving to Disk
5. Advice for Answering Long Text Questions
6. ERCAP error messages
7. Deleting a request

**FOR USERS**

- » Getting Help
- » Getting Started
- » Accounts & Allocations
  - Glossary
  - User Accounts
  - Allocations
    - Overview and Eligibility
    - Apply for Your First Allocation
    - Allocation Request Form (ERCAP)**
    - 2021 Call for Proposals
    - Allocation Proposal Deadlines
    - Request More Time
    - Allocation Reductions
    - Managing Your Allocation
    - DOE Allocation Managers
    - NESAP Application Process
    - Past Calls for Proposals
    - Awarded projects





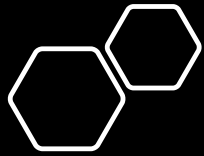
# The DOE Energy Sciences Network



# ESnet

ENERGY SCIENCES NETWORK

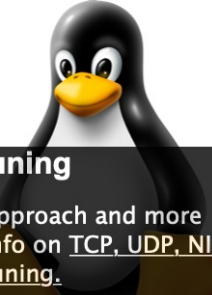
ESnet provides the high-bandwidth, reliable connections that link scientists at **national laboratories, universities, and other research institutions**. Funded by the DOE Office of Science, ESnet is managed and operated by the Scientific Networking Division at **Lawrence Berkeley National Laboratory**.



# Network Performance Knowledge Base

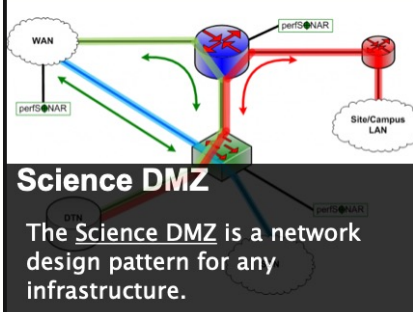
## ESnet Fasterdata Knowledge Base

An Expert Guide for End-to-End Performance Tuning, Tools and Techniques



### Linux Tuning

General approach and more specific info on [TCP](#), [UDP](#), [NIC](#), and [VM tuning](#).



### Science DMZ

The [Science DMZ](#) is a network design pattern for any infrastructure.



### Network Tuning

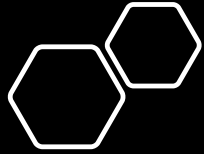
Fix [issues](#) with [TCP](#), firewalls, routers, switches, and more.

Data set size	
10PB	1,333.33 Tbps
1PB	133.33 Tbps
100TB	13.33 Tbps
10TB	1.33 Tbps

### Network Expectations

Information about benchmarks for networks and data transfer speeds.

100GB	13.33 Gbps
10GB	1.33 Gbps
1GB	133.33 Mbps



# Engagement and Performance Operations Center (EOPC)



<https://epoc.global>

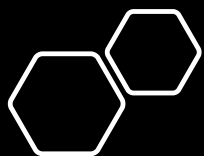
Established in 2018 with funding from NSF

Collaboration of Indiana U and U.S. DOE Energy  
Sciences Network (ES.net)



**ESnet**  
ENERGY SCIENCES NETWORK





# Engagement and Performance Operations Center (EOPC)

*EPOC provides researchers with a holistic set of tools and services needed to debug performance issues and enable reliable and robust data transfers.*

Roadside Assistance and consultation via a coordinated Operations Center to resolve network performance problems with end-to-end data transfers reactively

Application Deep Dive to work more closely with application communities to understand full workflows for diverse research teams in order to evaluate bottlenecks and potential capacity issues

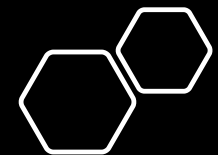
Network Analysis enabled by the NetSage monitoring suite to proactively discover and resolve performance issues

Provision of managed data services via support through the IU GlobalNOC and our Regional Network Partners

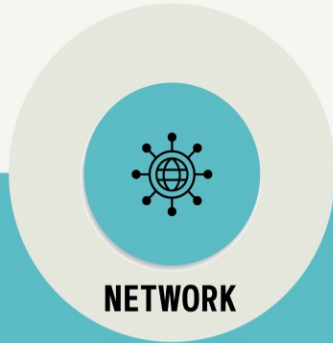
Coordinated Training to ensure effective use of network tools and science support



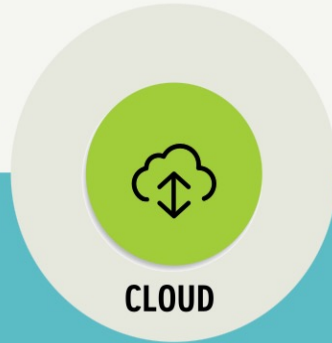
A not-for-profit US computer networking consortium led by members from the **research and education** communities, **industry**, and **government**.



High-performance  
Architecture & Services



Integrated Cloud  
Services



Community-developed  
Solutions



Collaborate with  
R&E Peers



320+  
HIGHER EDUCATION MEMBERS

44  
REGIONAL & STATE NETWORKS

750+  
EDUROAM SUBSCRIBERS

350+  
UNIVERSITY NET+ SUBSCRIBERS

50+  
INDUSTRY MEMBERS

1000+  
INCOMMON HIGHER EDUCATION, RESEARCH & CORPORATE PARTICIPANTS

750+  
NET+ CLOUD CONTRACTS

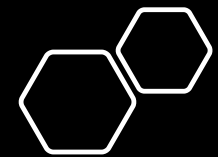
60  
AFFILIATE & GOVERNMENT MEMBERS

100+  
COUNTRIES & RESEARCH NETWORKS CONNECTIONS

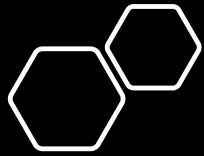
100,000+  
COMMUNITY ANCHOR INSTITUTIONS



# Open Science Grid



A National, Distributed Computing Partnership for Data-Intensive Research



Submit  
locally,  
compute  
globally



OSG Consortium  
founded in 2004



Created to facilitate  
data analysis from the  
Large Hadron Collider



Lends itself well to  
(High) Throughput  
Computing



Consists of over 25,000  
computers with over  
43,000 processors

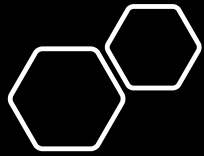


Funded by DOE as well  
as NSF

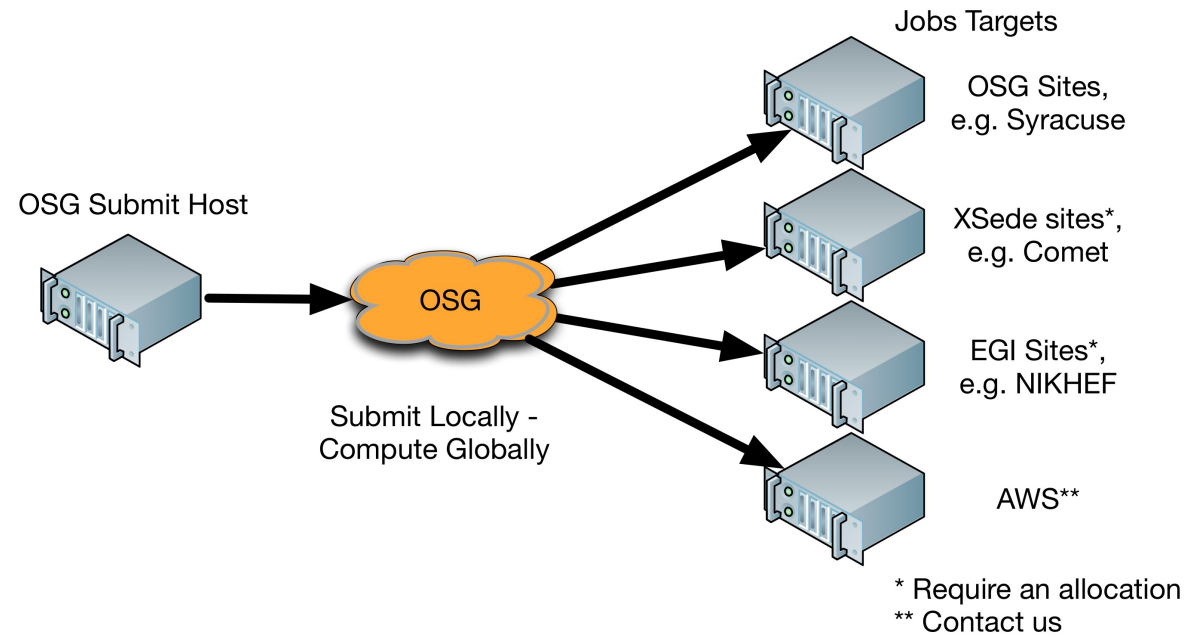


Employs the HTCondor  
software platform

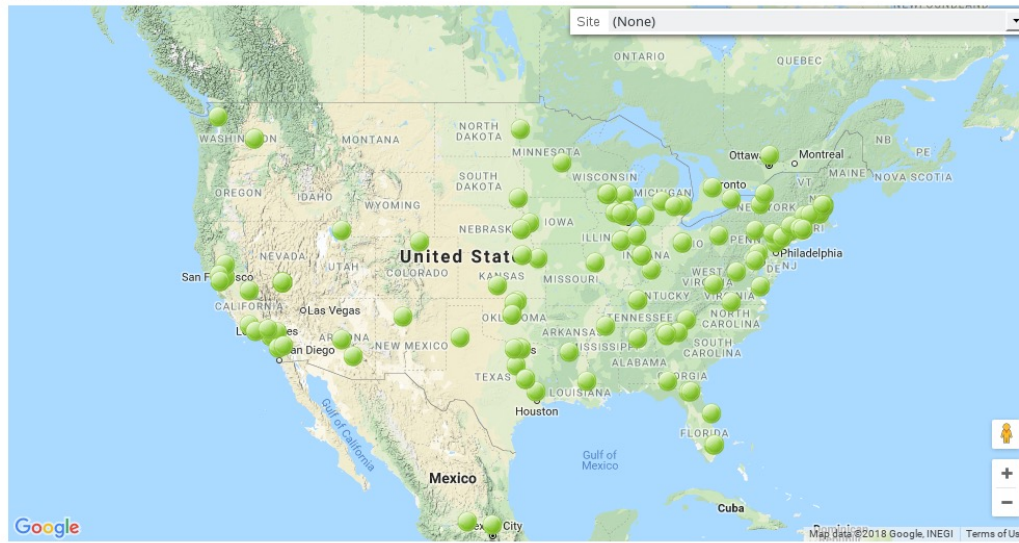




# How does it work?



Status Map **Jobs** CPU Hours Transfers TB Transferred



**In the last 24 Hours**

<b>346,000</b>	Jobs
<b>4,696,000</b>	CPU Hours
<b>7,784,000</b>	Transfers
<b>989</b>	TB Transfers

**In the last 30 Days**

<b>9,352,000</b>	Jobs
<b>129,774,000</b>	CPU Hours
<b>246,118,000</b>	Transfers
<b>23,888</b>	TB Transfers

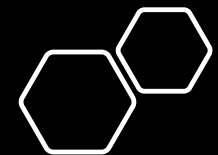
**In the last 12 Months**

<b>142,588,000</b>	Jobs
<b>1,585,993,000</b>	CPU Hours
<b>2,220,289,000</b>	Transfers
<b>195,000</b>	TB Transfers

OSG delivered across 126 sites

[Privacy policy](#)

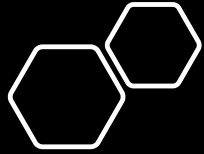
How distributed is it (as of 2018...)?



# ISGCI

SCIENCE GATEWAYS COMMUNITY INSTITUTE: CONNECTING PEOPLE AND  
RESOURCES TO ACCELERATE DISCOVERY BY EMPOWERING THE SCIENCE  
GATEWAY COMMUNITY





# Gateways

- 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.
- 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.

There are a lot of them.

Who have we worked with?  
65 projects engaged in 2.5 years



Let's look at one: Chem Compute

### Computational chemistry software for undergraduate teaching and research.

All without the hassle of compiling, installing, and maintaining software and hardware. Login or register at the top right to get full access to the system, or [learn more](#) about using Chem Compute in your class teaching.



#### Select a chemistry package:

##### GAMESS

The General Atomic and Molecular Electronic Structure System, a quantum chemistry package.

Use GAMESS

##### TINKER

A molecular dynamics package from the Jay Ponder Lab.

Use TINKER

##### JUPYTERHUB AND PSI4

Analyze data and run quantum calculations in Python

Use Jupyterhub / Psi4

##### NAMD

A molecular dynamics package from the Theoretical and Computational Biophysics Group at the University of Illinois Urbana Champaign

# Let's look at one: Chem Compute

Chem Compute GAMESS TINKER NAMD Psi4/Jupyter Instructors Datasets (beta) Contact Login / Register

HOME / GAMESS / SUBMIT [Hide Instructions](#)

## Instructions

(1) General Instructions

Instructions on how to build a molecule, submit a job, and view the results.

1. Make sure you are logged in. Registered users are allocated more computational power.
2. Click the next button to begin!

[Next](#)

### Choose your Molecule

You can draw your molecule in 2D or use the following options:

Search for a molecule:  
  
[Search](#)

Read Geometry From a Previous Job:  
  
[Load From Input](#) [Load From Output](#)

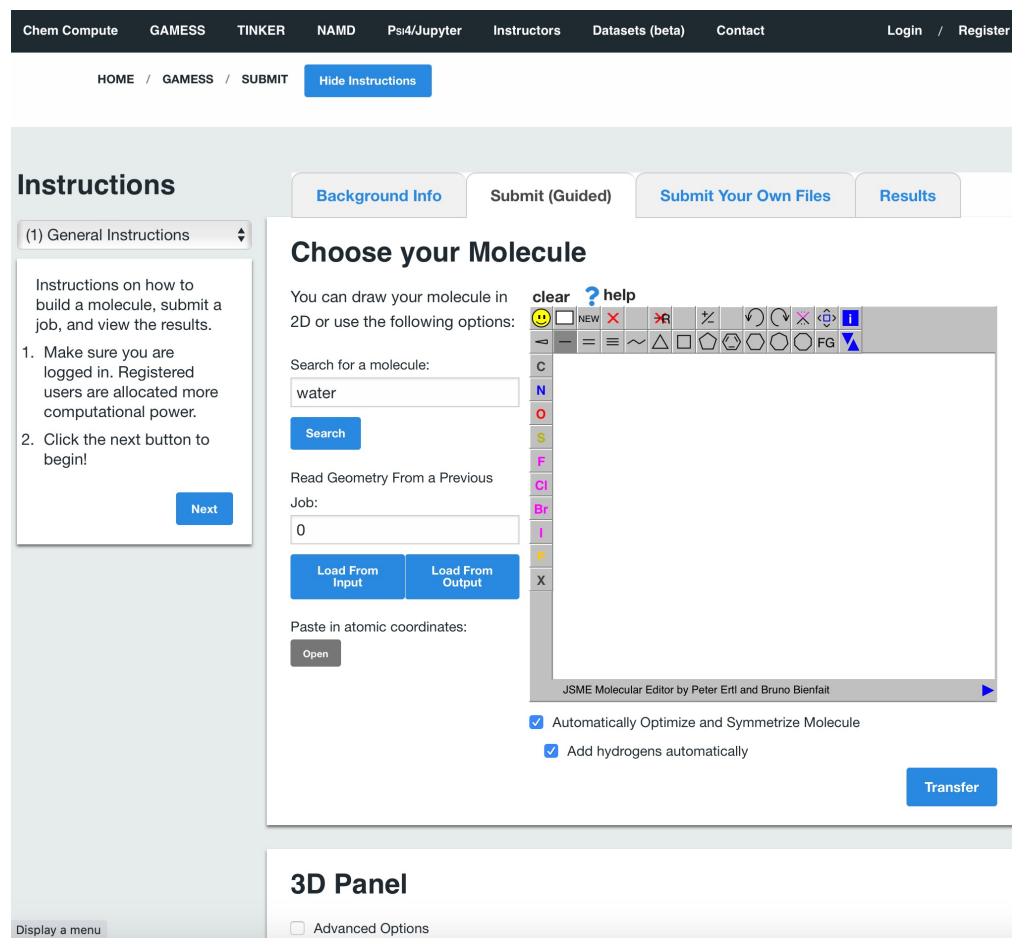
Paste in atomic coordinates:  
[Open](#)

Automatically Optimize and Symmetrize Molecule  
 Add hydrogens automatically

[Transfer](#)

### 3D Panel

Advanced Options



## (Some) International Organizations

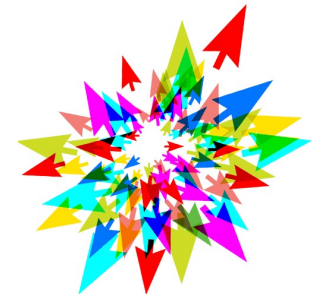
- The Partnership for Advanced Computing in Europe (**PRACE**) enables high-impact scientific discovery and engineering research and development across all disciplines by offering world class computing and data management resources and services.
- **G É ANT**: the pan-European data network for the research and education community.
- **Compute Canada** leads the acceleration of research and innovation by deploying state-of-the-art advanced research computing (ARC) systems, storage and software solutions for Canadian researchers and their collaborators in all academic and industrial sectors.



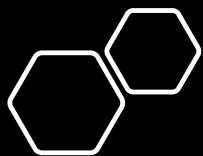
PARTNERSHIP FOR ADVANCED  
COMPUTING IN EUROPE



**compute** | **calcul**  
canada | canada





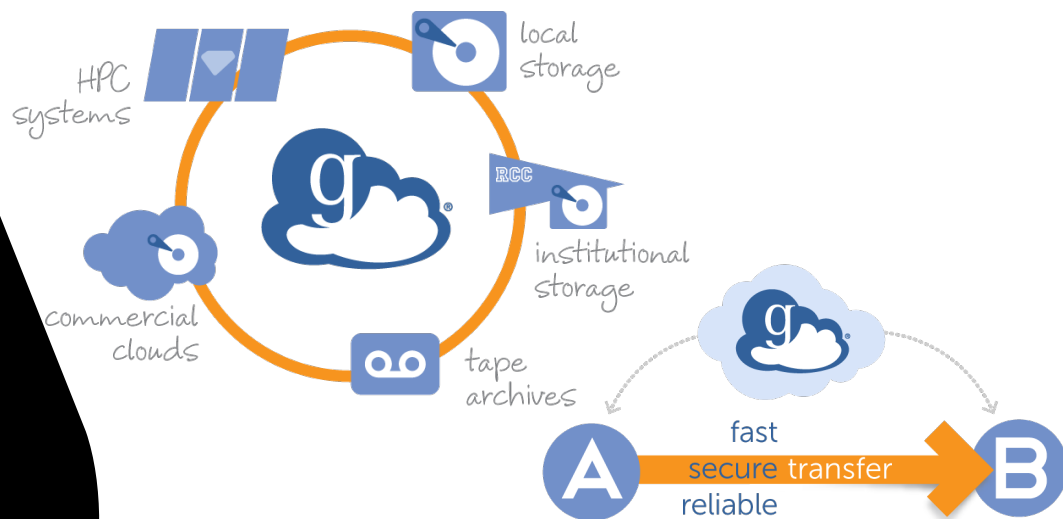


# Tools

- Globus
- XDMoD
- Open OnDemand
- Spack



# Spack

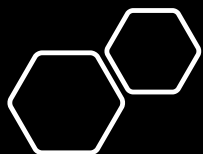


# XDMoD

METRICS ON DEMAND

**OPEN**

# OnDemand



Ask.Cyberinfrastructure.org

<https://ask.ci>

Public, searchable, archived Q&A  
platform for Research  
Computing

Joint project of Northeast  
Cyberteam Initiative at MGHPCC  
and Campus Champions



Welcome to Ask.CI! Our goal is to be the "go to" general Q&A platform for the global community of people who do research computing - researchers, facilitators, research software engineers, CI engineers, sys admins and others. We seek to streamline knowledge sharing and encourage self-service learning through centralized aggregation of experience, lessons learned and best practices, by encouraging a respectful discussion on research computing topics. Ultimately, our hope is that through frequent updates to relevant topics, this site will have the answers to most "of the moment" research computing questions asked by the community and these answers will show first in search engine results.

**Locales** are a place to get (and post) specific information about research computing at participating institutions and communities of practice. Pioneered by Stanford University, locales are now available for a growing list of schools and organizations around the US. [Learn more about Locales...](#)

**Please join our community!** Your participation, even posting just one or two questions or answers a year, will make a huge difference in helping us to reach this goal! We have a new users orientation on the first Friday of every month. [Learn more...](#)

all categories all tags Latest Categories Top

Topic	Replies	Views	Activity
<b>Softwares to support Social Scientists</b> Discussion Zone researcher, qow	2	213	6h
<b>Running COMSOL with MATLAB using LiveLink on SLURM cluster</b> Q&A connection, slurm, research-software, computational-chemistry, researcher, matlab, managing-sw, qow, 1 vote	0	144	15h
<b>Custom software stack environment for user (no sudo/root)</b> Discussion Zone research-software, administering-hpc, researcher	12	896	2d
<b>No Code or Low Code Solutions for HPC</b> Discussion Zone programming-for-hpc, researcher	4	197	2d
<b>Slurm vs PBS Pro (Community Edition)</b> Discussion Zone pbs, slurm, scheduler, systems	0	33	2d
<b>When using a GPU to accelerate NAMD, what are the drawbacks of using a single-precision GPU?</b> Q&A gpu, computational-chemistry, researcher, namd, simulation, 0 votes	2	91	3d

## Softwares to support Social Scientists

Discussion Zone qow, researcher

**S** schadalapaka 2 Apr 7

Hi,  
 Hope you're all doing well and are keeping safe.  
 At this point, many of our Social Scientists are exploring ways to move some of their projects online. What softwares for this purpose do your campuses support? There specifically seems to be an interest in the software called "millisecond" (<https://www.millisecond.com/products/inquisit6/web.aspx>). Do any of your campuses have a department/campus-wide license for this software? Also, if you have any recommendations for a free, open-source tools for data collection for online experiments, I would love to know your experiences in getting them to work.

Thanks!  
 Have a wonderful day ahead!  
 Regards,  
 Sarvani Chadalapaka  
 HPC Administrator  
 University of California Merced, Office of Information Technology

created last reply 2 217 3 2 2 S V  
 Apr 7 6h replies views users likes links

3 MONTHS LATER

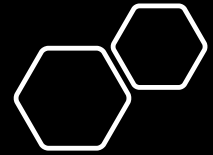
**CHannSoden** 20d

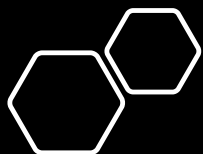
Hi Sarvani,  
 At Berkeley we've recently had some interest in [BEDCo](#) from public health and social science

Apr 7  
 1 / 3  
 Apr 7  
 6h ago

• Sites like Stack Exchange are dominated by the much larger enterprise IT sector.

• Research Computing questions benefit from **discussion**, not always just one answer.





Thank you!

Douglas M. Jennewein,  
Arizona State University,  
Campus Champions Leadership Team  
Douglas.Jennewein@asu.edu



CAMPUS  
CHAMPIONS

*With support from:*



**XSEDE**  
Extreme Science and Engineering  
Discovery Environment