

# *A Whirlwind Tour of Every Tool You Might Want to Know About*



**Douglas M. Jennewein, Arizona State University,  
Campus Champions Leadership Team  
All Champions Call  
September 15, 2020**

*With support from:*



**XSEDE**  
Extreme Science and Engineering  
Discovery Environment

But first...

This talk will (briefly) cover:

- Bridges
- Jetstream
- Stampede2
- Open Science Grid (OSG)
- Science Gateways
- EPOC
- Ask.ci

But first...

This talk will NOT cover:

- Frontera, Expanse, Voyager, Neocortex, Comet, Chameleon, CloudLab, other NSF / XSEDE systems
- NERSC / DOE Leadership Computing Systems

Only because:

1. Time
2. Availability
3. Doug doesn't know enough about all of them

# A word about allocations

The screenshot shows the XSEDE website's "Campus Champions Allocations" page. At the top, there is a dark blue header with the XSEDE logo and navigation links for "User Portal", "Web Site", and "Go to ▾". A search bar is also present. Below the header, the main content area has a light gray background. The title "Campus Champions Allocations" is centered at the top of the content area. On the right side, there is a sidebar titled "Campus Champions" with a vertical list of links: "Welcome", "Overview", "How does it work?", "For New Champions", "Champion Allocations", "Introductory Tutorials", and "Current Champions". The main content on the left includes sections for "Introduction" and "Starting an allocation request", along with instructions and a bulleted list of steps for requesting allocations.

## 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](#).

<https://www.xsede.org/web/campus-champions/ccalloc>



# 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



Carnegie Mellon University



University of Pittsburgh

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

# At a Glance

Launched in 2016

28,628 CPU cores

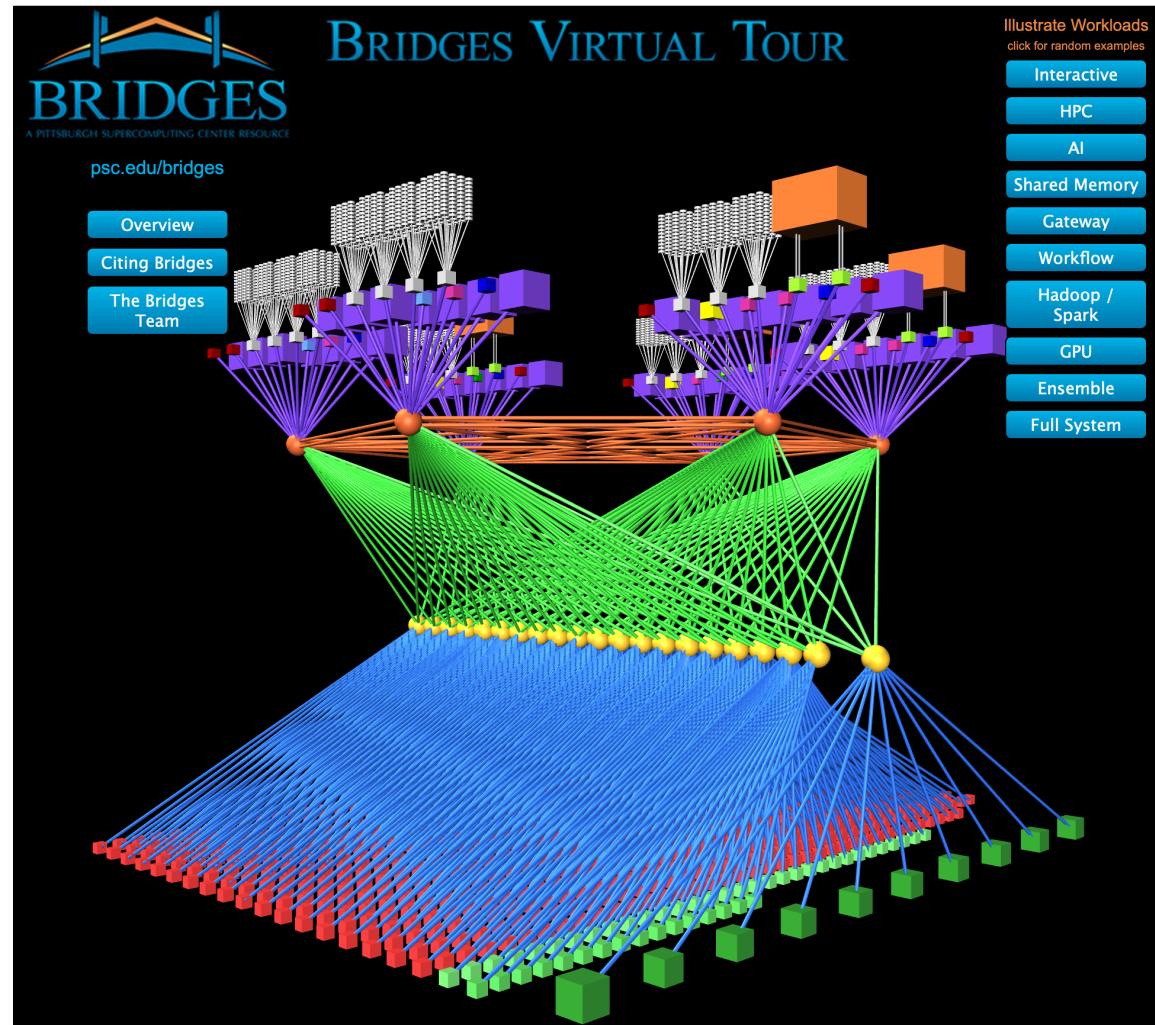
64 NVIDIA P100 GPUs

32 K80 dual GPUs

10PB persistent storage

7.3PB temporary storage

274TB memory



# One System, many modalities

Regular Memory (128GB)

Large Memory (3TB)

~~Insane~~ Extreme Memory (12TB) 😱

VMs

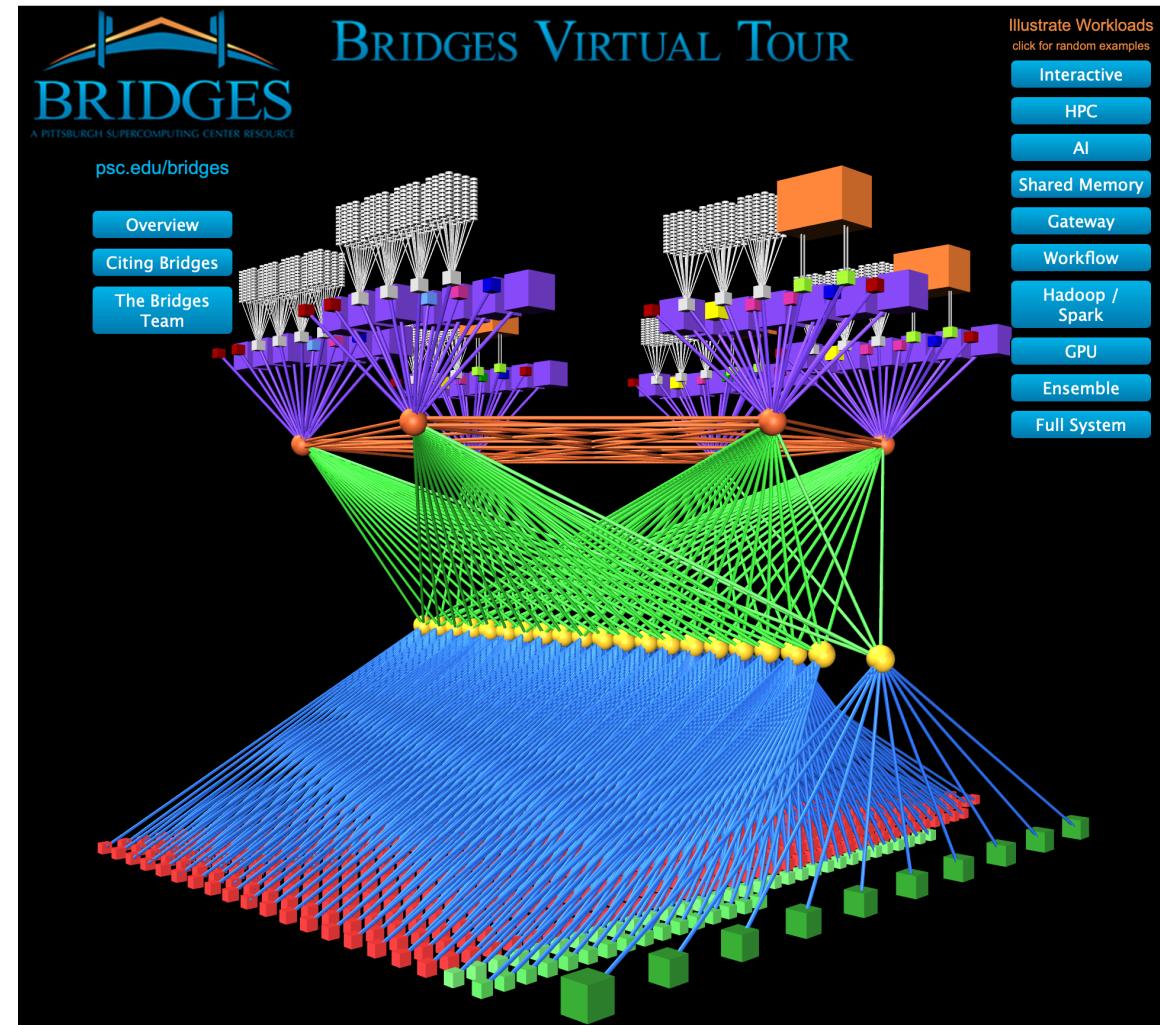
Containers

AI Frameworks

Interactivity

Web / Application Servers / Gateways

Database Servers



# 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.
- Bridges 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

- Dedicated database nodes power persistent relational and NoSQL databases
- Dedicated web server nodes
- OpenStack, KVM, Singularity
- Persistent community data collections: e.g. BLAST, ImageNet

Shared, dedicated, and persistent

# Bridges2 is coming this fall! (2020)

[www.psc.edu/bridges-2](http://www.psc.edu/bridges-2)

## Core Concepts

- Converged HPC + AI + Data
- Custom topology optimized for data-centric HPC, AI and HPDA
- Heterogeneous node types for different aspects of workflows
- CPUs and AI-targeted GPUS
- 3 tiers or per-node RAM: 256GB, 512GB, 4TB
- Extremely flexible software environment
- Community data collections & Big Data as a Service

## Innovation

- AMD EPYC 7742 CPUs: 64-core 2.25–3.4 GHz
- AI scaling to 192 V100-32GB 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, GPUDirect, SR-IOV, and data encryption
- Cray ClusterStor E1000 Storage System
- HPE DMF single namespace across disk and tape for data security and expandable archiving
- Converged HPC + AI + Data



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.

**Jetstream**

Dashboard Projects Images Help Admin jfischer ▾

### 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

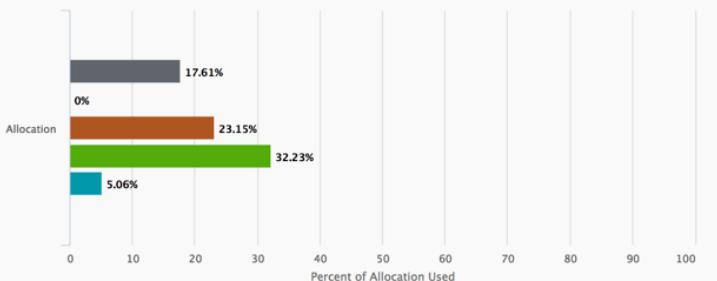
Modify your account settings, view your resource quota, or request more resources.

### Resources Used

Need more?

#### Allocation Source

TG-STA1100245 TG-ASC160018 TG-CDA160007 TG-TRA160003 TG-TRA160027



Allocation Source	Percent of Allocation Used
TG-TRA160003	32.23%
TG-CDA160007	23.15%
TG-TRA160027	17.61%
TG-STA1100245	5.06%
TG-ASC160018	0%

#### 10 Instances

active shutoff



#### 4 Volumes

available



#### Provider Resources

Jetstream – Indiana University Jetstream – TACC



Provider	CPU Usage
Jetstream – Indiana University	9.09%
Jetstream – TACC	0%

©2017 Jetstream-Cloud [Feedback & Support](#)

SEARCH

FAVORITES (0)

MY IMAGES (0)

MY IMAGE REQUESTS

TAGS

## Image Search

Search across image name, tag or description

Showing 57 of 57 images

### Featured Images

	<b>Centos 7 (7.2) Development GUI</b> Jan 13th 17 03:21 by jfischer	Imported Application - Centos 7 (7.2) Development GUI <a href="#">CentOS</a> <a href="#">development</a> <a href="#">Featured</a> <a href="#">gui</a> <a href="#">IRODS</a>	
	<b>BioLinux 8</b> Jan 2nd 17 03:34 by jfischer	Based on Ubuntu 14.04.3 -Trusty Tahr - server - cloudimg - **REQUIRES m1.small instance ... <a href="#">bioinformatics</a> <a href="#">desktop</a> <a href="#">Featured</a> <a href="#">gui</a> <a href="#">m1_small</a> <a href="#">Ubuntu</a> <a href="#">x2go</a>	
	<b>Ubuntu 14.04.3 Development GUI</b> Jan 2nd 17 01:24 by jfischer	Based on Ubuntu 14.04.3 Development Patched up to date as of 12/15/16 Base Ubuntu 14.04.3 ... <a href="#">desktop</a> <a href="#">development</a> <a href="#">Featured</a> <a href="#">gui</a> <a href="#">IRODS</a> <a href="#">Ubuntu</a> <a href="#">vnc</a>	
	<b>Intel Development (CentOS 7)</b> Nov 30th 16 12:04 by jfischer	Intel compilers and development environment *REQUIRES a m1.small or larger VM to la ... <a href="#">CentOS</a> <a href="#">desktop</a> <a href="#">development</a> <a href="#">Featured</a> <a href="#">gui</a> <a href="#">Intel</a> <a href="#">m1_small</a> <a href="#">vnc</a>	
	<b>R with Intel compilers (CentOS 7)</b> Nov 30th 16 11:53 by jfischer	R with Intel compilers built on CentOS 7 (7.3) ** Requires m1.small or greater sized VM * ... <a href="#">CentOS</a> <a href="#">desktop</a> <a href="#">development</a> <a href="#">Featured</a> <a href="#">gui</a> <a href="#">Intel</a> <a href="#">m1_small</a> <a href="#">vnc</a>	
	<b>Galaxy Standalone</b> Nov 15th 16 04:49 by admin	Galaxy 16.01 Standalone - based on Ubuntu 14.04.4 LTS This is a standalone Galaxy server ... <a href="#">community-contributed</a> <a href="#">Featured</a> <a href="#">m1_large</a> <a href="#">Ubuntu</a>	

jetstream

Dashboard Projects Images Help Admin jfischer ▾

**JLF Test**

**RESOURCES**

**Instances**

- Name
- Build - R with Intel compilers (CentOS 7)
- Test 4 - JLF Private
- KVM image to build

**Volumes**

- Name
- IntelCompiler
- IntelCompiler

**Images**

You have not added any images to this project.

**Links**

You have not added any links to this project.

**Launch an Instance / Basic Options**

**Basic Info**

Instance Name: R with Intel compilers (CentOS 7)

Base Image Version: 1.14

Project: JLF Test

**Resources**

Allocation Source: TG-CIE170025

Provider: Jetstream - Indiana University

Instance Size: m1.tiny (CPU: 1, Mem: 2 GB, Disk: 8 GB)

Allocation Used: 0% of 140000 SUs from TG-CIE170025

Resources Instance will Use

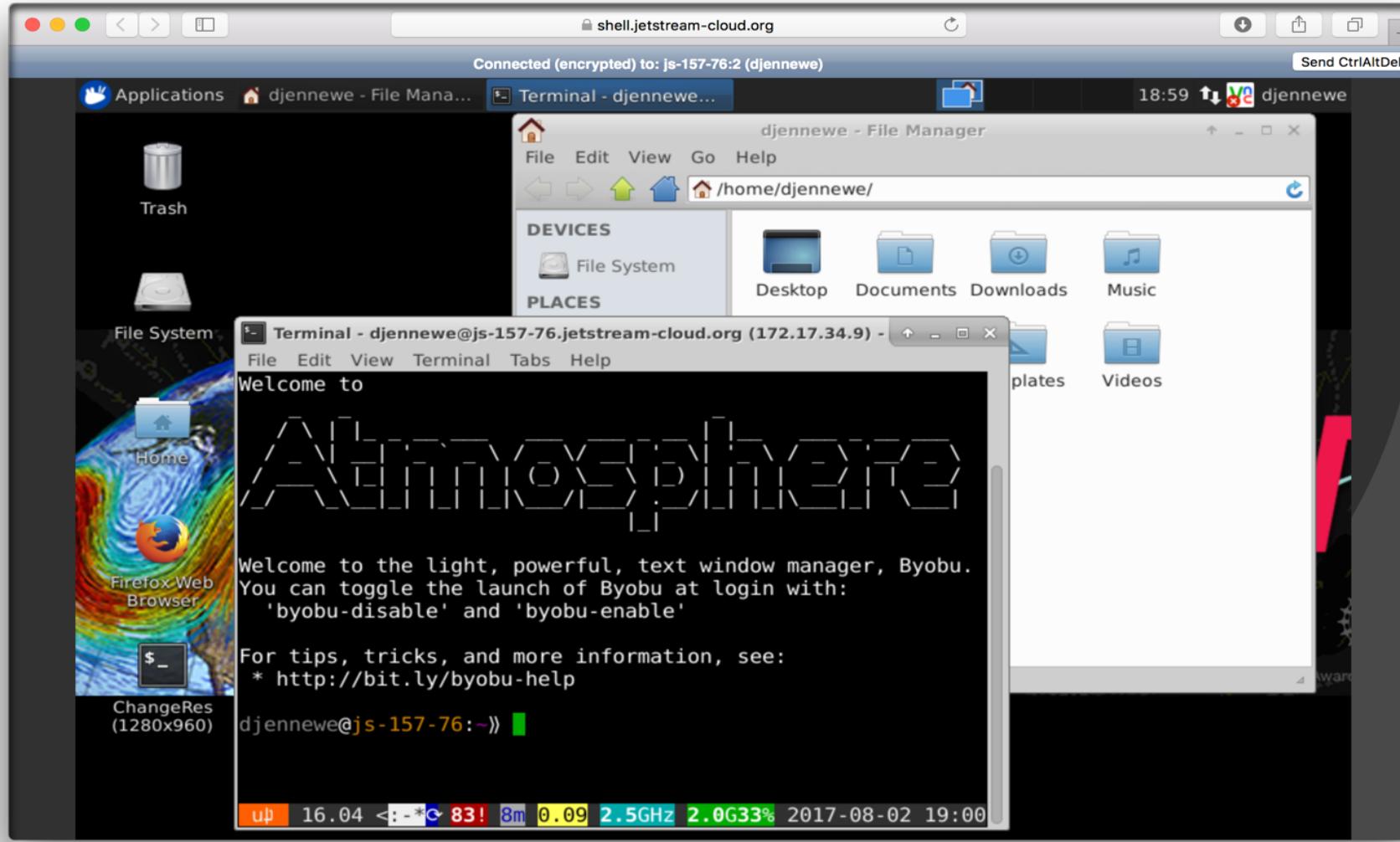
A total 14 of 132 allotted CPUs

A total 38 of 360 allotted GBs of Memory

**OPTIONS ▾**

**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

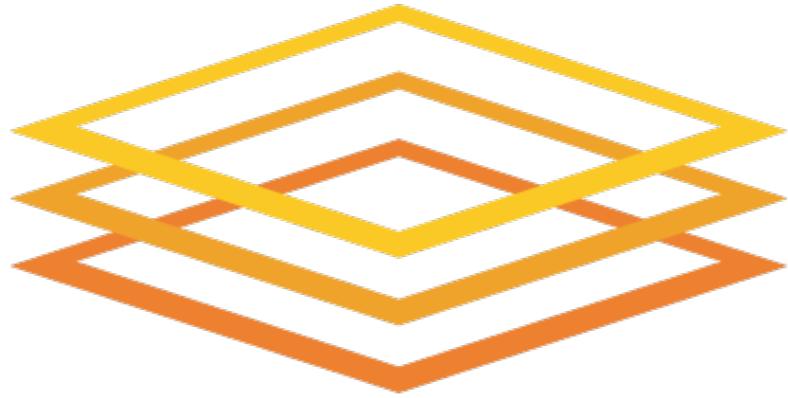
- Unified instance management
- Multi-instance launch



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!

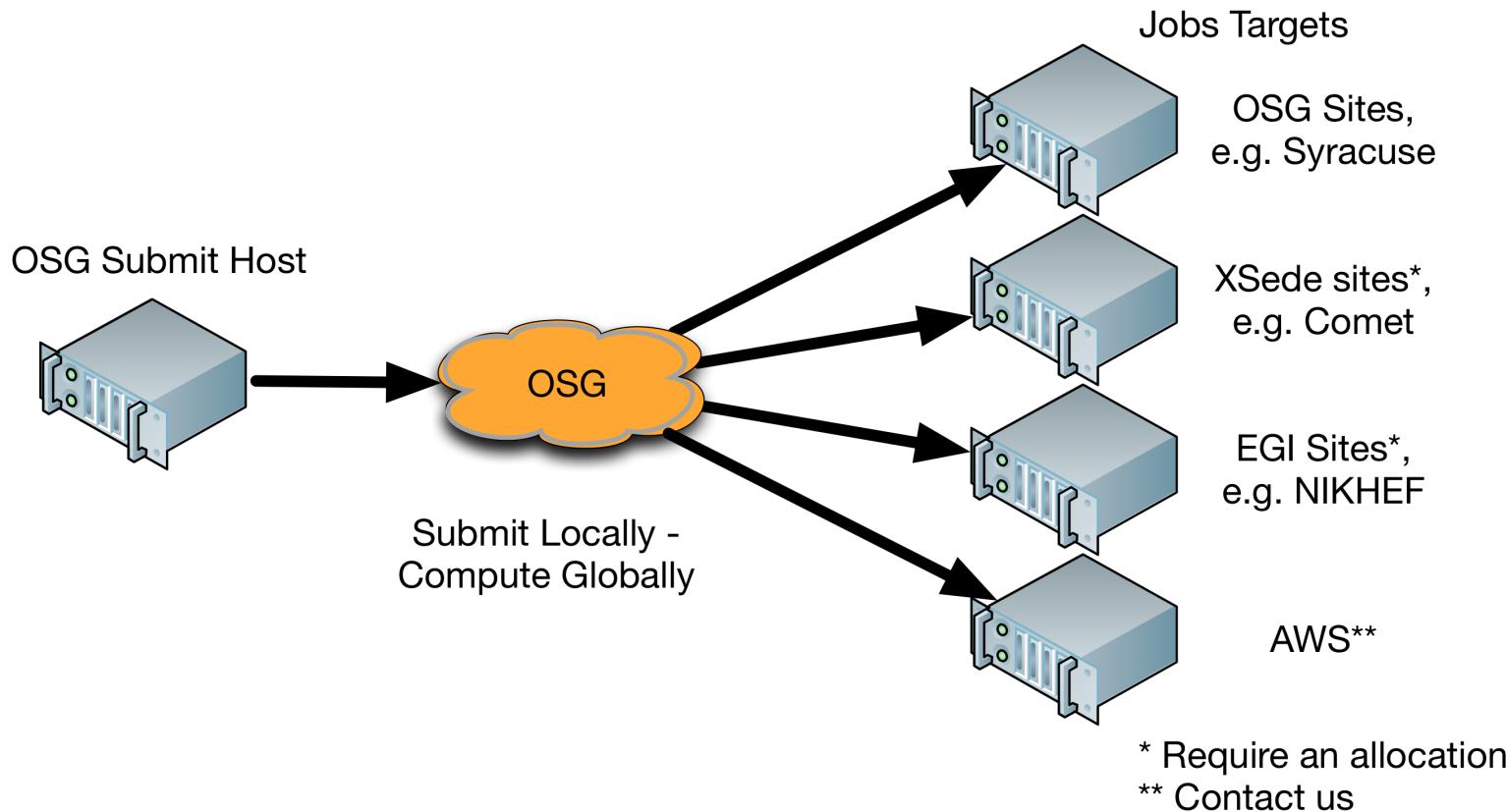


# Open Science Grid

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?



Open Science Grid

A national, distributed computing partnership for data-intensive research

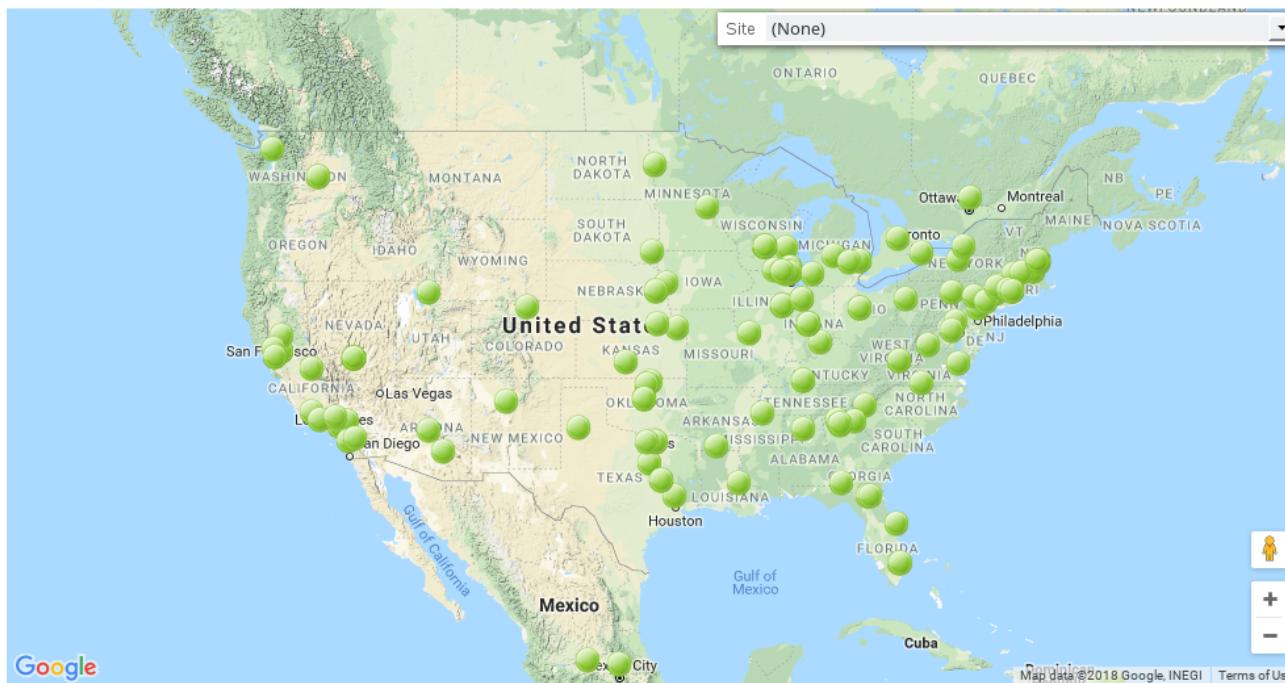
Status Map

Jobs

CPU Hours

Transfers

TB Transferred



In the last 24 Hours

346,000 Jobs

4,696,000 CPU Hours

7,784,000 Transfers

989 TB Transfers

In the last 30 Days

9,352,000 Jobs

129,774,000 CPU Hours

246,118,000 Transfers

23,888 TB Transfers

In the last 12 Months

142,588,000 Jobs

1,585,993,000 CPU Hours

2,220,289,000 Transfers

195,000 TB Transfers

OSG delivered across 126 sites

[Privacy policy](#)

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



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

# Gateways

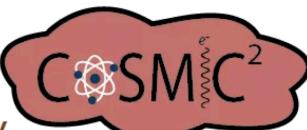
Science Gateways simplify access to computing resources by **hiding infrastructure complexities**.

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.

Who have we worked with?

65 projects engaged in 2.5 years



Coastal Emergency Risks Assessment  
ADCIRC Coastal Circulation and Storm Surge Model + SWAN Wave Model



<https://sciencegateways.org/consulting/clients>

There are a lot of them.

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

HOME /

**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

[Use NAMD](#)

# 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:

clear ? help

Search for a molecule: water

Search

Read Geometry From a Previous Job: 0

Load From Input   Load From Output

Paste in atomic coordinates: Open

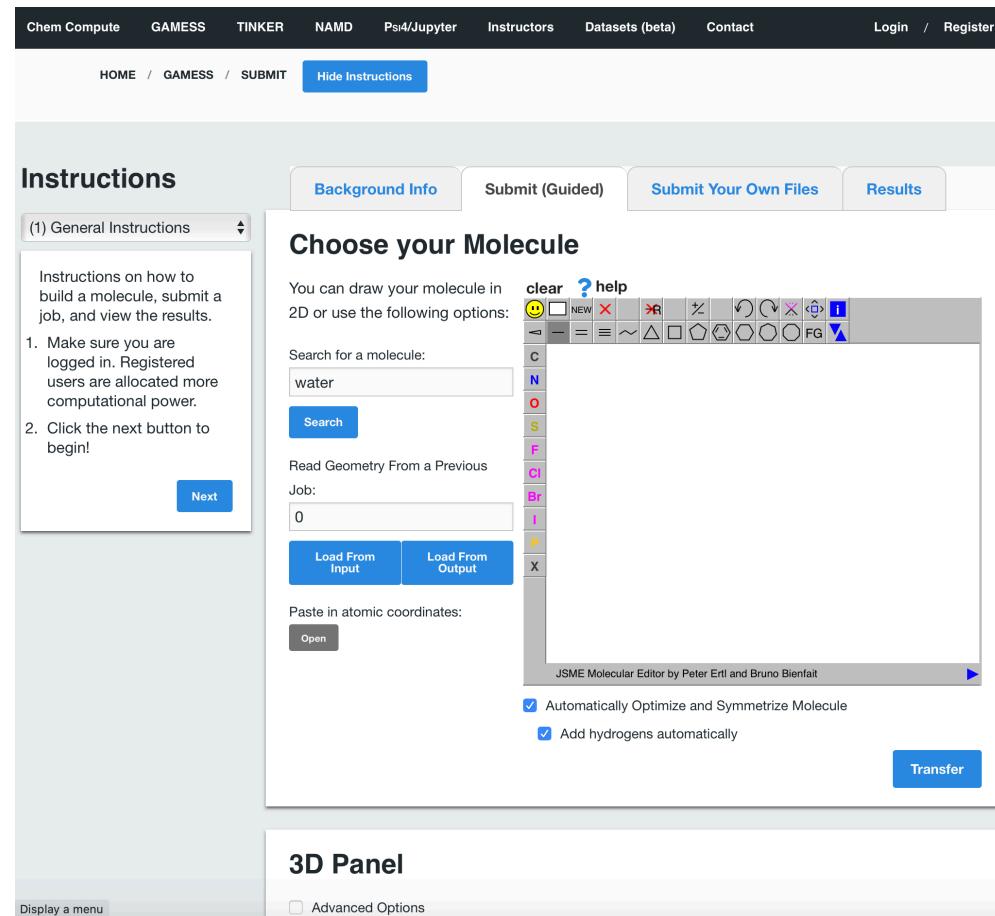
JSME Molecular Editor by Peter Ertl and Bruno Bienfait

Automatically Optimize and Symmetrize Molecule  
 Add hydrogens automatically

Transfer

## 3D Panel

Display a menu   Advanced Options



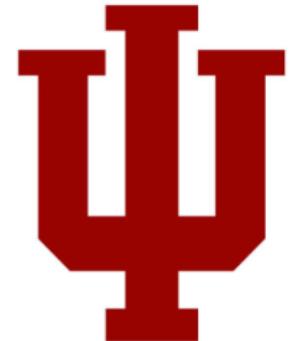
# Let's look at one: Chem Compute

# 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)



*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





- Public, searchable, archived Q&A platform for Research Computing
- Joint project of Northeast Cyberteam Initiative at MGHPCC and Campus Champions
- Launched at PEARC18
- Discourse platform

Ask.Cyberinfrastructure.org  
<https://Ask.CI>

**ASK.CYBERINFRASTRUCTURE**

Home Sign Up Log In

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

- Launched 2018
- Weekly page views: 16K-20K
- Inception to date: 295K page views (as of 7.26.20)
- Users: 440
- Unique Institutions: over 220

## Softwares to support Social Scientists

Discussion Zone qow, researcher



schadlapaka

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 replies	217 views	3 users	2 likes	2 links		
Apr 7	6h							

3 MONTHS LATER



CHannSoden

20d

Hi Sarvani,

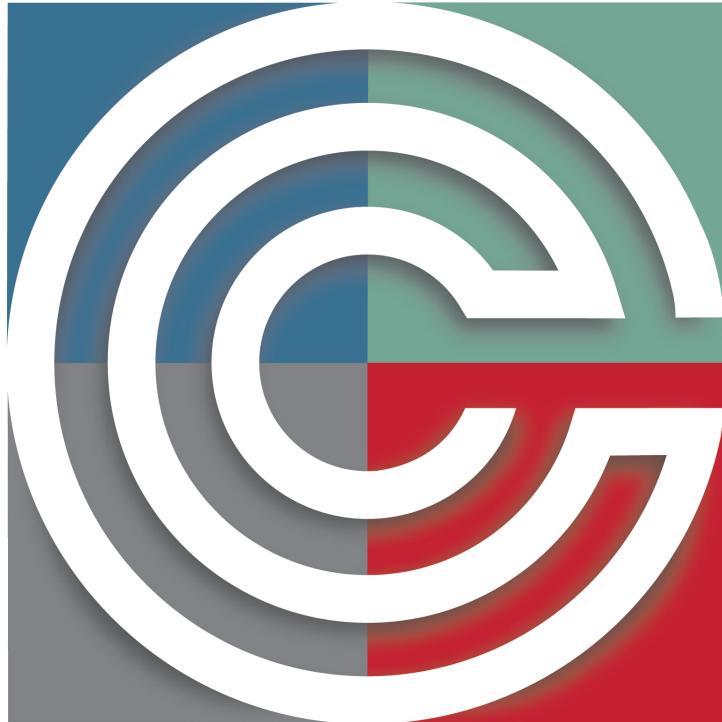
At Berkeley we've recently had some interest in REDCap [1](#) from public health and social science

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.



CAMPUS  
CHAMPIONS

# Thank you!

**Douglas M. Jennewein,  
Arizona State University,  
Campus Champions Leadership Team**

*With support from:*



**XSEDE**

Extreme Science and Engineering  
Discovery Environment