



#### **Ohio Supercomputer Center**

An OH·TECH Consortium Member





Ohio St.

### Computing Services to Accelerate Research and Innovation

An introduction to OSC services





#### Kate Cahill Education & Training Specialist

"OSC is here to empower your research."



### Outline

- What is OSC?
- Overview of Services
  - Hardware Overview
  - Data Storage Systems
  - Software Overview
  - Upcoming services
- OSC Usage and Case Studies
- Research Partnership
- Getting Started at OSC
  - Getting access
  - Learning how to use OSC resources





"640K ought to be enough for anybody." – Not Bill Gates



### **About OSC**

- Founded in 1987
- Statewide resource for all universities in Ohio
  - high performance computing services
  - computational science expertise
  - " ... propel Ohio's research universities and private industry to the forefront of computational based research."
- Funded through the Ohio Department of Higher Education
- Reports to the Chancellor
- Located on OSU's west campus
- Fiscal agent is OSU





### **The OH-TECH Consortium**



**Ohio Supercomputer Center** provides high performance computing, software, storage and support services for Ohio's scientists, faculty, students, businesses and their research partners.



**OARnet** connects Ohio's universities, colleges, K-12, health care and state and local governments to its high-speed fiber optic network backbone. OARnet services include co-location, support desk, federated identity and virtualization.



**OhioLINK** serves nearly 600,000 higher education students and faculty by providing a statewide system for sharing 50 million books and library materials, while aggregating costs among its 90 member institutions.



### **Service Catalog**



**Cluster Computing** A fully scalable center with mid-range machines to match those found at National Science Foundation centers and other national labs.



Research Data Storage High-performance, large capacity data storage spaces along with others that are perfect for a wide variety of research data.



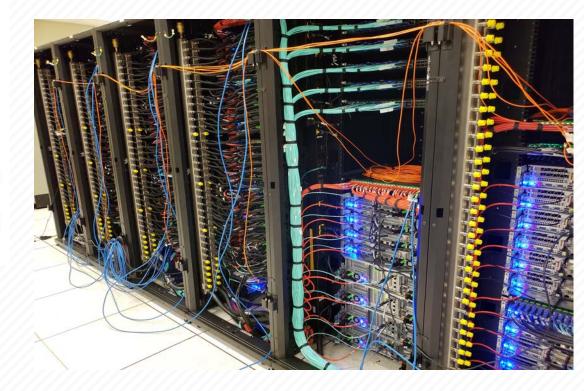
Education High performance computing and networking resources come together to create an exciting and innovative teaching and research environment.



Web Software Development Our expert web development team helps you create custom web interfaces to simplify the use of powerful HPC resources.



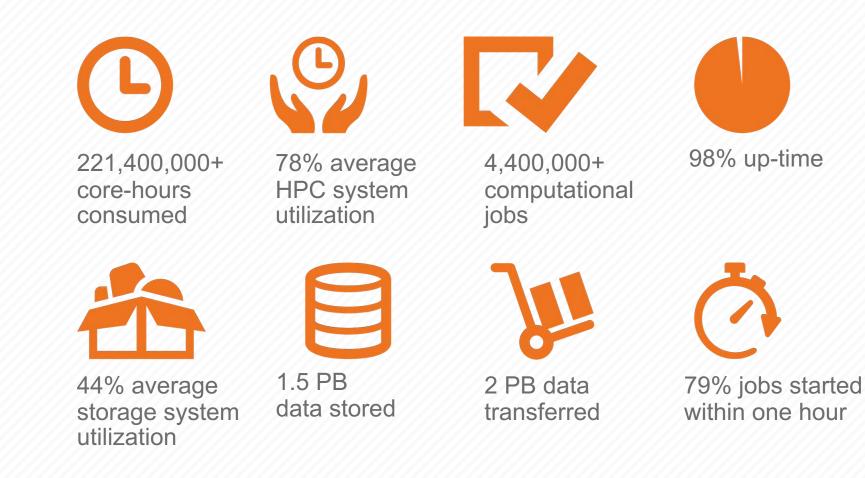
Scientific Software Development Deep expertise in developing and deploying software that runs efficiently and correctly on large scale cluster computing platforms.





# **Production Capacity**

CY2017







#### **Hardware Overview**

"To err is human, but to really foul things up you need a computer." – Paul Ehrlich

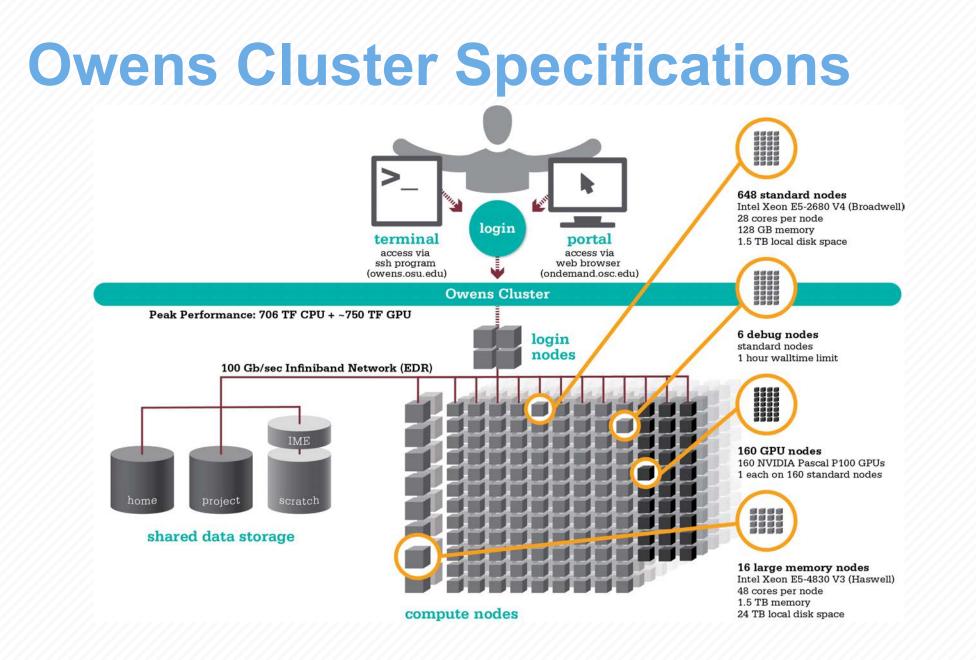


### System Status (2019)

SYSTEMS	Ruby	Owens	Pitzer
Date	2014	2016	2018
Cost	\$1.5 million	\$7 million	\$3.35 million
Theoretical Perf.	~144 TF	~1600 TF	~1300 TF
Nodes	240	824	260
CPU Cores	4800	23392	10560
RAM	~15.3 TB	~120 TB	~ 70.6 TB
GPUs	20 NVIDIA Tesla K40	160 NVIDIA Pascal P100	64 NVIDIA Volta V100
		Total compute: ~3,044 TF	

STORAGE	Home	Project	Scratch	Tape Library
Capacity	0.8 PB	3.4 PB	1.1 PB	7+ PB
Current utilization Feb, 18	47%	48%	59%	47%







### New HPC Cluster "Pitzer"

- Named after Russell M. Pitzer
  - Emeritus professor of chemistry at The Ohio State University
  - Instrumental in founding both OSC and OARnet
- Goals
  - Complement existing systems
  - Replace Oakley with a petaflop class system
- Timeline
  - System delivery August 15, 2018
  - Full production November 2018
  - Oakley decommissioning Dec 2018



### **Pitzer Cluster**

#### **Characteristics relative to Oakley**

- Delivers 8x the processing power (1,300 vs 154 TF)
- Costs 15% less (\$4M vs \$3.35M)
- Provides 25% more cores (10,560 vs 8,304)
- Has 2X the memory (70.6Tb vs 33.4TB)
- Uses 20% less power

#### **Highlights**

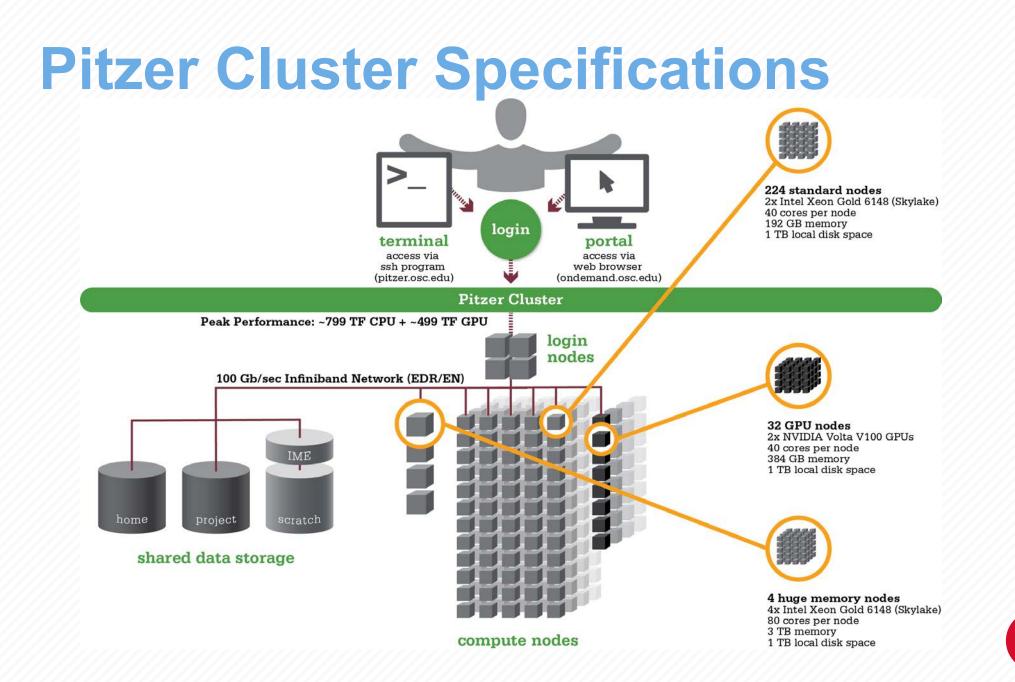
- 10,560 processor cores, ~1.3 petaflop peak
- Latest generation: SkyLake processors, 100Gb InfiniBand
- Warm water cooling supports high density, increased performance and efficiency

#### **3 Types of Resources and Example Workload**

- Standard compute (224 nodes) / Modeling and simulation for industry
- GPU (32 nodes) / Machine learning, artificial intelligence (AI)
- Large memory (4 nodes) / Genomics Sequence Assembly





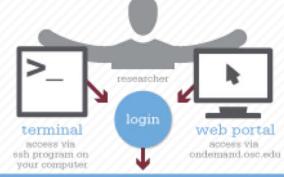


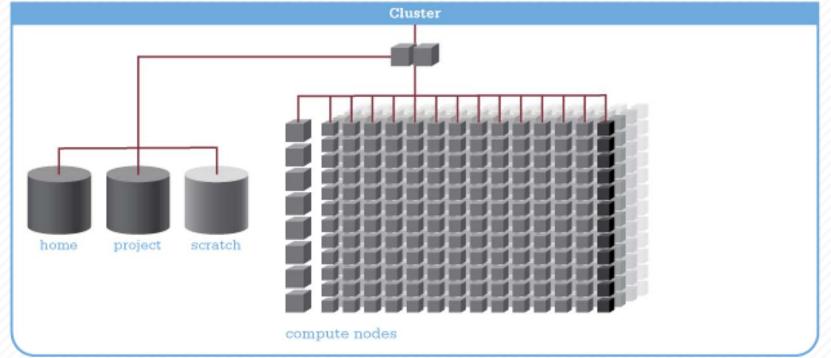


"War is ninety percent information." - Napoleon Bonaparte



### Four different file systems







### **Filesystem Overview**

- Home
  - Store files for individual users
  - Backed up daily
- Project
  - Large scale persistent storage
  - Available to Project Pls by request
  - Shared by all users on a project, backed up daily

- Scratch
  - Store large input or output files for HPC simulation or analysis
  - Faster I/O than Home or Project
  - Temporary storage, not backed up
- \$TMPDIR
  - Storage on compute nodes, for use during a job
  - Results must be copied to another location
  - All data purged when job quits





### **Software Overview**

"It works on my machine." - unknown



c+132 meanzilla the ansys \_\_in Software Resources for OSC Clients astac gaac amber sp Slat Isp aw siesta acca , ecel aces2 cml lammps Parsec am inca can enzo POP as COMSO

- More than 150 software packages,
  - https://www.osc.edu/resources/available\_software
- Types of Software include compilers, development tools, numerical libraries, applications
- Mix of ISV, free and open source packages



### **Overview – software development tools**

- Compilers: Intel, gnu, PGI
- MPI: MVAPICH, IntelMPI, OpenMPI
- OpenMP: supported by Intel, gnu and PGI compilers
- GPU: latest CUDA, OpenACC (PGI compilers)
- Performance and debug tools: Arm, Intel and opensource tools
- Containers: singularity to run docker containers, with support for GPU



# If OSC doesn't have the software you need?

- List of applications can be found at Software page: http://www.osc.edu/supercomputing/software/
- Commercial/Licensed software
  - Fill out a request form (see our FAQ)
  - SUG will consider it
- Open-source software
  - You can install it yourself in your home directory
  - If there's enough demand, we can install it for shared use
- Have your own license?
  - Contact OSC Help





### **Upcoming Services**

"In God we trust. All others must bring data." – W. Edwards Deming



### **Client Portal Project**

### Replacement for my.osc.edu

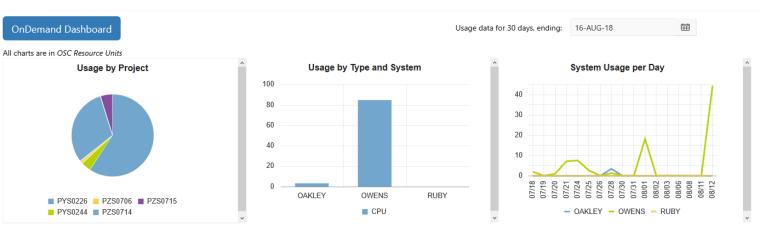
- Friendly user testing started on August 17
- Scheduled go-live for all clients on October 23

#### New reports.osc.edu

 Provides OSC staff with robust client usage and billing reporting capabilities

#### Project Dashboard Admin × Project × Individual × Software

#### Project Dashboard



#### oject Summaries

Project	Status	Title	Principle Investigator	Usage (RU)	Balance (RU)	Storage (TB)	More
PYS0226	ACTIVE	PG RESEARCH	Alan Chalker	52.41	71295	1.0635	Usage Details
PYS0244	ACTIVE	COMMERCIAL PROJECT: IN STATE	Alan Chalker	3.57	99186.4405	-	Usage Details
PZS0694	ACTIVE	OPEN ONDEMAND	Alan Chalker	0	4948.602	-	Usage Details
PZS0685	ACTIVE	PRIVATE 2018	Alan Chalker	0	1991201	-	Usage Details
PAW0001	ACTIVE	AWSMDEV	Alan Chalker	0	99175.0748	-	Usage Details
PAN0014	ACTIVE	TEST FOR BASIL	Alan Chalker	0	49975.6687		Usage Details
PZS0666	ACTIVE	EMC2 VFT HPC WEB APPLICATION COLLABORATION	Alan Chalker	0	303.1967	-	Usage Details
PND0017	DISABLED	NDEMC PROJECT	Alan Chalker	0	5000	-	Usage Details



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### **Data Focused Projects**

#### **Protected Data Environment**

- Unique resource supporting HIPAA, ITAR, or other sensitive data sets
- Initial requirements gathering (OSU Wexner Medical Center, Nationwide Children's Hospital)
  - Provide standard OSC environment with security assurances, assistance with data management plans
  - Collect requirements for different services for new communities

#### **Research Data Archive**

- Simplify data management plans for sponsored research
- Provide publishing and other abstraction capabilities
- Additional off-site copy of data for resiliency/availability

#### **Project file system expansion**

- Increase space for metadata, 2-3B files/directories (1B today)
- Slower tier of storage for infrequently accessed files



### **Other Capital Projects**

#### **Production infrastructure refresh**

- "C20" HPC cluster (replaces the Ruby cluster)
- Storage upgrades
  - Additional fast tier storage
  - Other performance/capacity upgrades
  - Tape media capacity expansion
- Hardware to support protected data environment and research data archive
  - May include "Cloud" resources
- Other EOL hardware





### HPC Usage and Case Studies

"The difference between us and a computer is that, the computer is blindingly stupid, but it is capable of being stupid many, many million times a second." – Douglas Adams



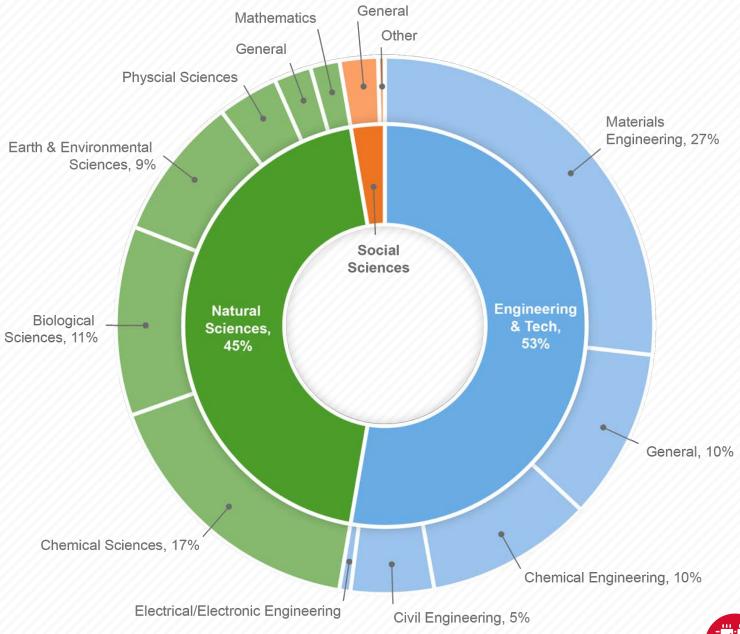
## **Client Services**

CY2017





### Usage by Field of Science





### **OSC Client Distribution by University (CY2017)**

Institution	Active Users
Bowling Green State University	31
Bluffton University	7
Cedarville University	1
Cleveland State University	18
Case Western Reserve University	30
Kent State University	21
Kenyon College	1
Miami University	27
Oberlin College	2
Ohio Dominican University	1
Ohio Northern University	1
Ohio University	45
The Ohio State University	996
University of Akron	40
University of Cincinnati	162
University of Dayton	27
University of Toledo	22
Wittenberg University	1
Wright State University	11
Youngstown State University	9



## Academic Course Enrollment

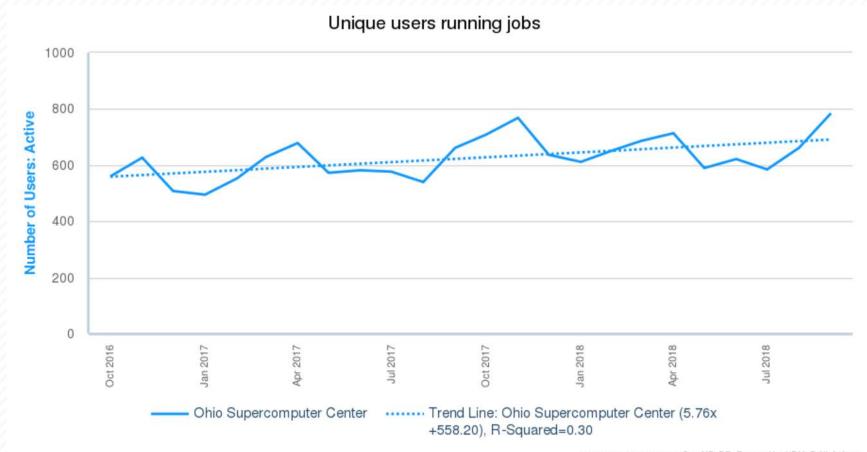
Department		
Bluffton Mathematics	9	
OU Chemical & Biomolecular Engineering		
OU Chemistry & Biochemistry	2	
OSU Materials Science & Engineering	39	
OSU Chemical & Biomolecular Engineering	19	
OSU Materials Science & Engineering	16	
OSU Materials Science & Engineering	6	
OSU Computer Science & Engineering	30	
OSU Computer Science & Engineering	21	
OSU Evolution, Ecology, & Organismal Biology	18	
OSU Computer Science & Engineering	3	
OSU Evolution, Ecology, & Organismal Biology	12	
OSU Biostatistics	3	
OSU Chemistry & Biochemistry	28	
OSU Computer Science & Engineering	34	
OSU Computer Science & Engineering	75	
OSU Geography	13	

Department	
OSU Computer Science & Engineering	49
OSU Computer Science & Engineering	5
OSU Chemistry	400
OSU Chemistry	14
OSU Chemistry	10
OSU Chemistry	129
OSU Chemistry	105
OSU Chemistry	10
Akron Mechanical Engineering	12
UC Electrical Engineering & Computer Systems	18
UC Physics	23
UC Electrical Engineering & Computer Systems	63
UC Electrical Engineering & Computer Systems	60
UD Electrical & Computer Engineering	13
UD Electrical & Computer Engineering	14
Toledo Chemistry	16

#### 1,279 total students



### **Unique Users**



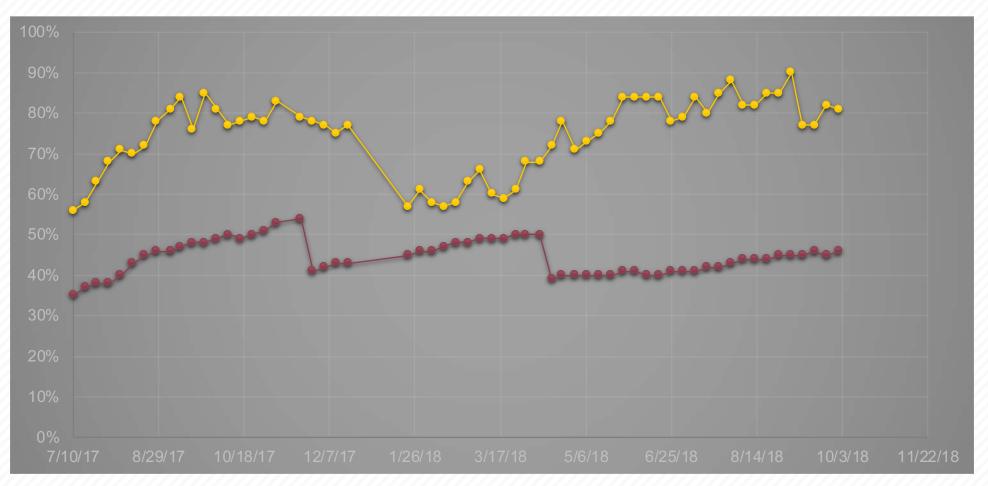
2016-10-01 to 2018-10-01 Src: HPcDB. Powered by XDMoD/Highcharts



OSC System Core Hours CY2017	IS	Downtimes: 6.4M Dedicated Queues: 7.5M Unschedulable: 31.4M Commercial: 28.7M	Hospital: 0.5M Consumer Goods: 0.6M Energy Tech Company: 0.6M
Oakley: 73.0M		OSC Internal: 2.3M	BGSU: 8.2M Ohio U.: 9.0M U. C.: 10.0M
Ruby: 42.1M			CWRU: 16.2M
Owens: 205.1M	Total: 320.2M	Academic: 185.0M	OSU: 132.5M
			Other: 5.8M
		Unused: 58.9M	



### **Project & Scratch Storage Utilization**





# Why would HPC be necessary for your work?

- Your simulations or analyses take too long on your personal computer
- The size of your data is too large to be contained (storage) or accessed (memory) on your computer
- You would like to free up your own system to do other tasks
- You need particular software for your work







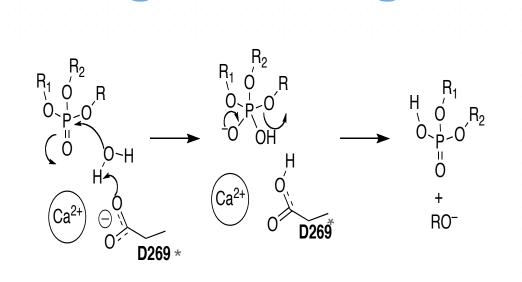
#### Mapping

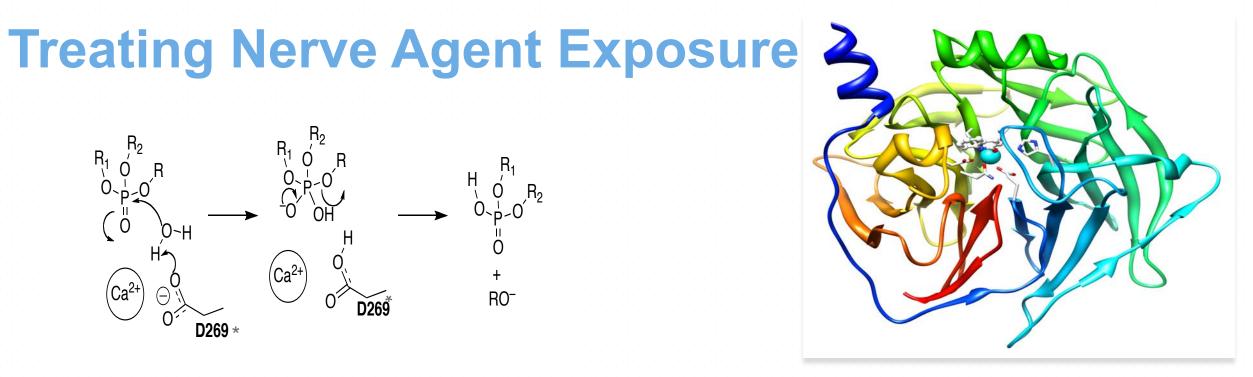
Researchers who normally use OSC systems to enhance satellite images of glaciers turned their technology to disaster relief assistance following Nepal's April 2015 earthquake

PI: Ian Howat, Ohio State University

Source: NSF Office of Polar Programs







#### **Treating Nerve Agent Exposure**

With the power of OSC computing services, a team studies how to capture and destroy organophosphorus nerve agents using modified proteins.

PI: Christopher Hadad, Ohio State University





"Alone we can do so little; together we can do so much." – Helen Keller



## **Research Partnership Opportunities**

- Letters of commitment sufficient resources needed for your project
- Boilerplate text regarding computing and storage facilities and data retention policy
- Quotes for specialized services such as: dedicated computing resources, large amounts of storage, HPC consulting
- Expertise in areas such as: scientific software development, web software development and virtual environments by collaborating as co-investigators or senior personnel.
- Opportunities for Outreach/Broader Impact activities with OSC's K12 summer educational programs
- Review of proposals for research computing infrastructure or research software development





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- Two-week residential program for high school students
- 16-20 participants each year since 1989
- Students solve complex problems under mentorship of OSC faculty clients

## Young Women's Summer Institute

- One-week residential program for middle school girls
- 16 participants each year since 2000
- Promotes STEM skills under mentorship of middle school teachers





### **Getting Started at OSC**

"If you were plowing a field, which would you rather use? Two strong oxen or 1024 chickens?" - Seymour Cray



# Who can get an OSC project?

- Academic project
  - Principal investigator (PI) must be a full-time faculty member or research scientist at an Ohio academic institution
  - PI may authorize accounts for students, post-docs, collaborators, etc.
  - Classroom projects are also available
  - No cost<sup>\*\*</sup> to Ohio academic users
- Commercial projects
  - Commercial organizations may purchase time on OSC systems





## **Allocations and Charges**

- Charges are in terms of resource units
- Resource units
  - OWENS 1 resource unit (RU) = 10 CPU hours
  - RUBY 1 resource unit (RU) = 20 CPU hours
  - Pitzer 1 resource unit (RU) = TBD
  - CPU hour = walltime x (total # of cores requested)
- Project receives an allocation of RUs
- Jobs are charged to a project



#### Requesting a New Projectmy.osc.edu

- Startup grant
  - One per PI per lifetime
  - Provide contact info, institution, department
  - 5000 RUs
- Additional allocations for a project
  - Submit a proposal for more RUs
    - Standard: 10,000
    - Major: 30,000
    - Discovery: >30,000
  - Peer-reviewed
  - Grants awarded by Statewide Users Group (SUG)
- Classroom accounts



# **Fee Structure Transition**

#### **FY19 Plan details**

- FY19 rate of \$0.075 / RU for cycles > 10K RUs per project; no storage charges
- Projected to provide the \$1M needed to cover the OSC budget gap
- FY19 MOUs signed by the 6 biggest universities (OSU, BGSU, OU, UA, CWRU, UC: signing in process)
- OSC will be reaching out to other schools (e.g. Cleveland State) that have low expenses projected (\$5K or more for the year).

#### Implementation

- Initial OSC Pricing Committee meeting March 12<sup>th</sup>, recent meeting on June 1st
- Implementation issues are being worked out, including an updated allocations process, regular institutional usage reporting, and refund policies
- Discussions are beginning with the OSC pricing committee regarding a revised model for FY20 that will likely include other charges / services





#### **Onboarding new users**

"After growing wildly for years, the field of computing appears to be reaching its infancy." – John Pierce



# **Beyond Command Line Access**

OSC OnDemand ondemand.osc.edu

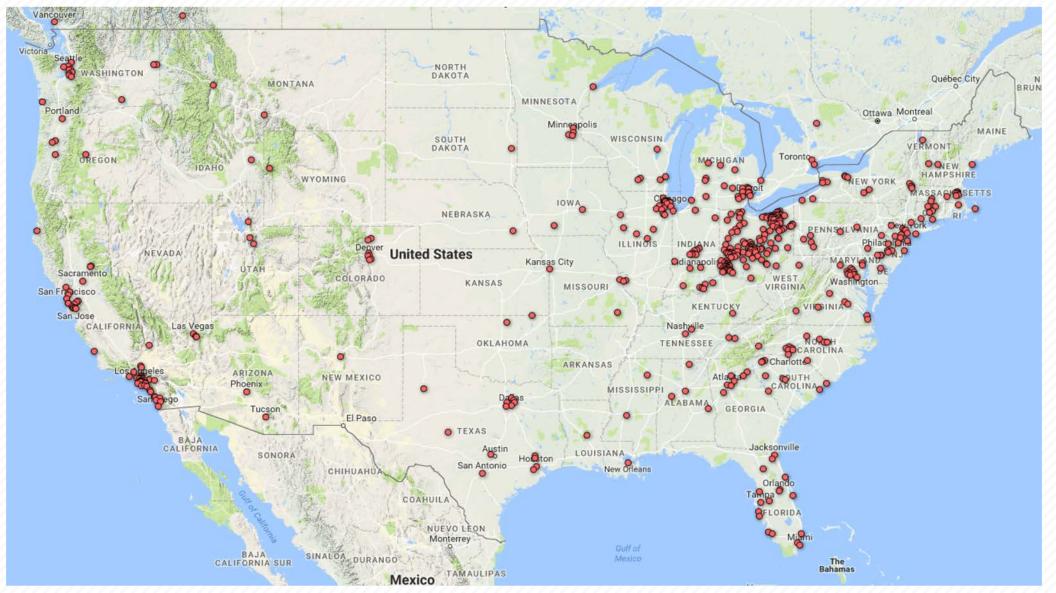
- 1: User Interface
  - Web based
    - Usable from computers, tablets, smartphones
    - Zero installation
  - Single point of entry
    - User needs three things
      - ondemand.osc.edu
      - OSC Username
      - OSC Password
    - Connected to all resources at OSC

- 2: Interactive Services
  - File Access
  - Job Management
  - Visualization Apps
    - Desktop access
    - Single-click apps (RStudio, Jupyter, Matlab, Abaqus, Ansys, Comsol, Paraview)
  - Terminal Access
    **Tutorial available at**
  - osc.edu/ondemand



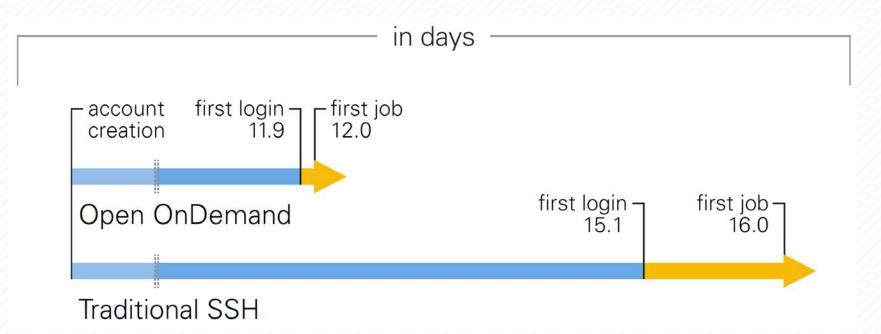
## **Web-based US Logins**

**CY2017** 



# **Open OnDemand Project**

• New OSC OnDemand users start faster than ssh users: first login & job



- Open OnDemand currently in use / evaluation at 30+ organizations
- Open OnDemand 2.0: NSF CSSI award, Jan'19 Dec'22, \$3.5M



# **Training & Outreach Activities**

#### Recent

- 5 classroom presentations on OSC services
- HPC Carpentry workshop at OSU/Physics
- OSC Big Data
- Several XSEDE events

#### Ongoing

- M-F 4-5PM in Pomerene Hall
- Every other Tuesday afternoon at Research Commons – remote consultations available

#### Upcoming

- Wright State: Intro presentation, Oct 18<sup>th</sup>
- Wright State: hands-on workshop, Oct 30th
- Bowling Green: Nov 1<sup>st</sup>
- OSC: Big Data workshop, Nov 28<sup>th</sup>
- CWRU, UC, OU, and OSU all planned for the spring semester



# New Intro to OSC materials

https://khill42.github.io/OSC\_IntroHPC/

- Highlights OnDemand for OSC access
- Always available training
- Continually being updated and improved
- Based on HPC/Data carpentry materials

#### Introduction to High Performance Computing

Advanced computing skills and the capacity to analyse large datasets are key for many researchers across a variety of disciplines. This workshop is designed to enable researchers to use High Performance Computing (HPC) systems to improve their research efficiency.

By the end of this workshop, students will know how to:

- Use the UNIX command line and the OnDemand web portal to connect to a remote computer.
- Navigate and interact with files using the UNIX command line.
- Work interactively with programs on an HPC setup.
  Execute scripted workflows on an HPC.
- Submit and manage jobs to an HPC using a job scheduler.

#### # Prerequisites

This workshop is designed for those with NO PRIOR EXPERIENCE. Students will need their own laptop computer. Students will need access to their institutional HPC.

#### Schedule

	Setup	Download files required for the lesson
00:00	1. Introduction to HPC	What is High Performance Computing?
		Why should I be using High Performance Computing for my research?
		Don't I need to know how to program to use High Performance Computing?
00:10	2. Connect to the HPC	How do I connect to an HPC system?
00:25	3. Basic UNIX Commands	What is the syntax of UNIX commands?
		How do I navigate the file system?
		How do I transfer files to HPC?
		How do I interact with files on the HPC?
00:55	4. Using a cluster: Introduction	What is a cluster?
		How does a cluster work?
		How do I log on to a cluster?
01:15	5. Using a cluster: Scheduling jobs	What is a scheduler and why are they used?
		How do we submit a job?

## Academic Community Engagement

- Deepen outreach to Ohio universities
- Empowers local support staff to work directly with clients
- Projects created at UC, OSU, Miami, and CWRU



### Statewide Users Group (SUG)

- The Statewide Users Group (SUG) is made up of OSC users
  - Provides program and policy advice to OSC
  - Meets twice a year
- Standing committees
  - Allocations
  - Software and Activities
  - Hardware and Operations
- Get involved!
  - Next meeting will be in March/April



# Get your questions answered

FAQs: <u>https://www.osc.edu/resources/getting\_started/supercomputing\_faq</u> HOW TOs: <u>https://www.osc.edu/resources/getting\_started/howto</u>

New User Guide: https://www.osc.edu/resources/getting\_started/new\_user\_resource\_guide

Updated presentations: <u>https://www.osc.edu/~kcahill/NewUser</u>

Office Hours and contacting OSC support staff:

go.osu.edu/rc-osc Tuesdays 1-3 p.m. or Weekdays 4-5 p.m. at OSU Pomerene Hall

Email help: <u>oschelp@osc.edu</u>

System updates

- Read Message of the Day on login
- Follow @HPCNotices on Twitter





#### OH·TECH

Ohio Technology Consortium A Division of the Ohio Department of Higher Education



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f facebook.com/ohiosuperco mputercenter w osc.edu

B oh-tech.org/blog

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