

# Ohio Supercomputer Center

An **OH·TECH** Consortium Member

Computing Services to Accelerate Research and  
Innovation

Kate Cahill

Education & Training Specialist

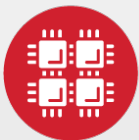


# Outline

- Overview
  - What is OSC?
  - HPC Concepts
  - Hardware Overview
- How to use our systems
  - User Environment
  - Storage
  - Batch Processing
  - Policies
- OSC News







# Ohio Supercomputer Center

An **OH·TECH** Consortium Member

## What is the Ohio Supercomputer Center?

# 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.



**eStudent Services** provides students increased access to higher education through e-learning and technology-enhanced educational opportunities, including virtual tutoring.



**Research & Innovation Center** will operate, when opened, as the proving grounds for next-generation technology infrastructure innovations and a catalyst for cutting-edge research and collaboration.



# Ohio Innovates with the World





# 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



# Empowering Clients: Organizational Impact CY2015

## Client Services



25 Ohio-based universities



32 companies



1,267 clients



124 trainees



10 educational opportunities



451 awards made



459 projects served



19 academic courses used OSC's supercomputers

## Production Capacity



161,000,000+ core-hours consumed



4,000,000+ computational jobs



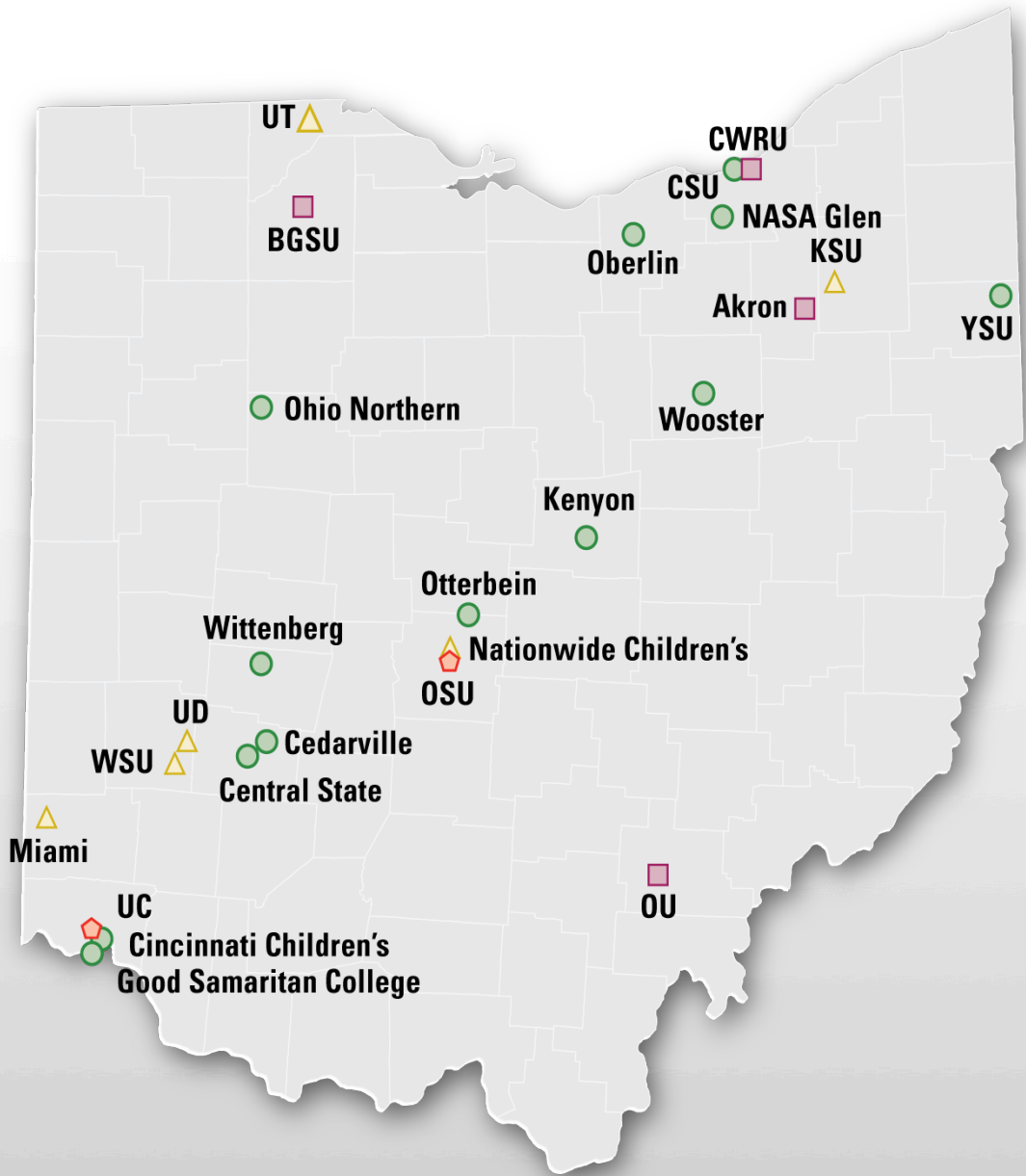
842 TB data stored



99.7% up-time (target: 96%)

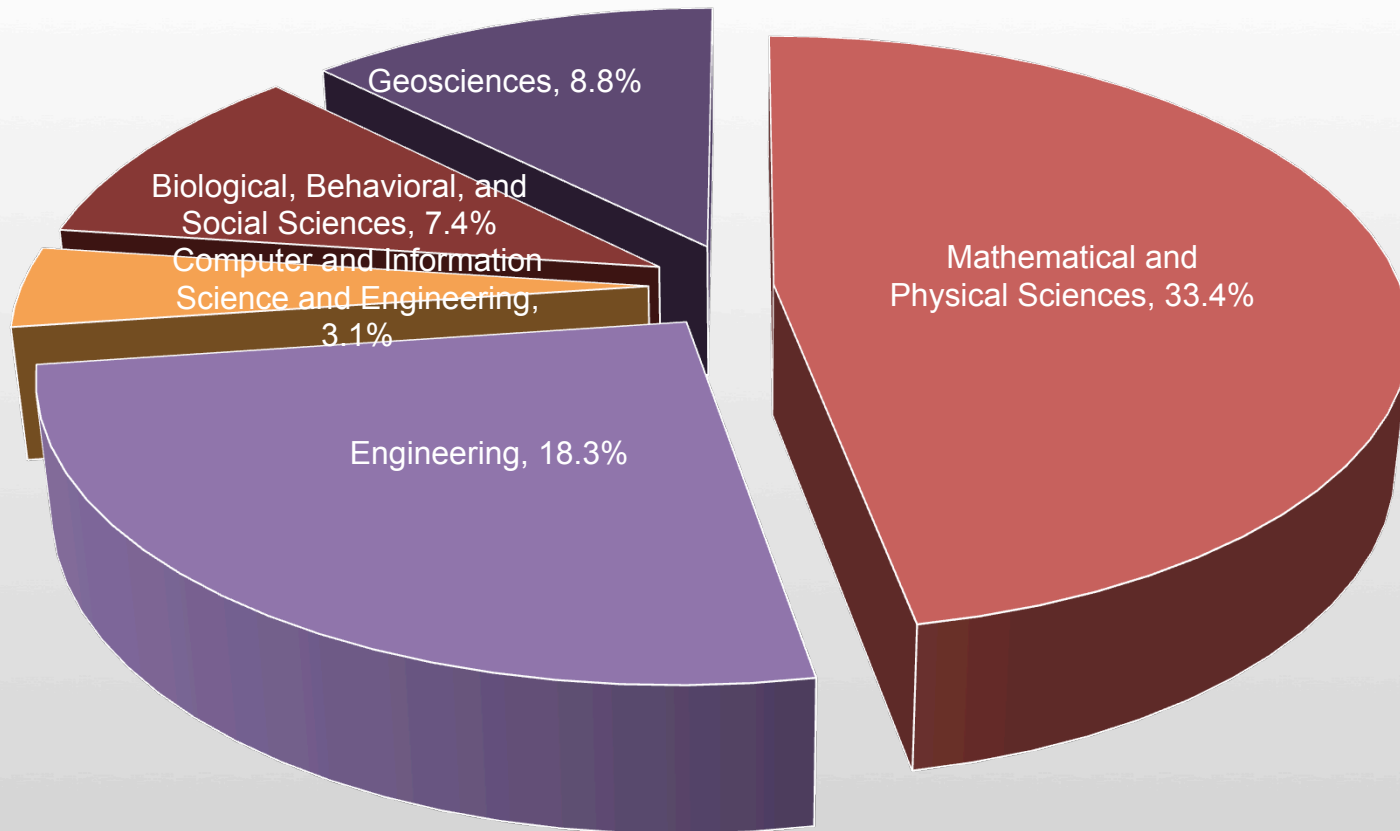


# Active Awards Total: 459



# Computing Resource Usage by Field of Science (FoS)

## Aggregate Hours



# OSC Service Catalog

## Cluster Computing

- High Performance Computing
- High Throughput Computing
- Data-intensive Computing

## Research Data Storage

- Project Storage
- Archival Storage

## Client Services

- 24x7 Call Center
- Level 2 Engineering Support

## Client Facilitation

- Consultation (in-person and online)
- Training and Education
- Classroom accounts

## Scientific Software Development

- Software Development
- Software Parallelization

## Web Software Development

- Software Development
- Software Consulting

## Partner on Proposals

- Cyberinfrastructure solutions
- Modeling & simulation for industry

## Visualization & Virtual Environments

- Visualization Services
- Virtual environments (DSL)





# HPC Client Services

- Technical Assistance
  - Help desk and basic consulting
  - Contact by phone or email ([oschelp@osc.edu](mailto:oschelp@osc.edu))
- Facilitation
  - Meet with OSC staff to discuss your research needs
  - Get recommendations on services, connections to subject matter experts, and specialized projects initiated
- Project Administration
  - Manage allocations
  - Add/Remove authorized users
  - Utilization reports
- Training
  - Usually three workshops per semester on a variety of topics
- Advanced consulting
  - Code parallelization & optimization
  - Software development, algorithm research
- Website
  - [www.osc.edu/supercomputing](http://www.osc.edu/supercomputing)





## What can OSC provide you?

- You can complete your research for less cost.
- You can do more science for the same cost.
- You can get to solution faster.



# What can OSC provide you?

- “Capability computing” (High Performance Computing)
  - Computation too large to run on laptop/desktop
- “Capacity computing” (High Throughput Computing)
  - Takes too long on laptop, need to make many runs
- Data Analytics
  - Massive memory requirements
- Access to licensed software
  - Have academic licenses for many commercial packages
- Expertise, collaboration
  - Parallel computing, algorithms, web portals, etc.

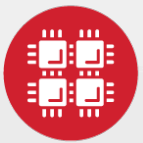




# Statewide Licensed Software

- Use the software in your lab or office
  - Connect to license server at OSC
- Software available
  - Altair Hyperworks
  - Totalview Debugger
  - Intel Compilers, Tools, Libraries
  - Portland Group Compilers
- Contact OSC Help
  - Provide your IP address





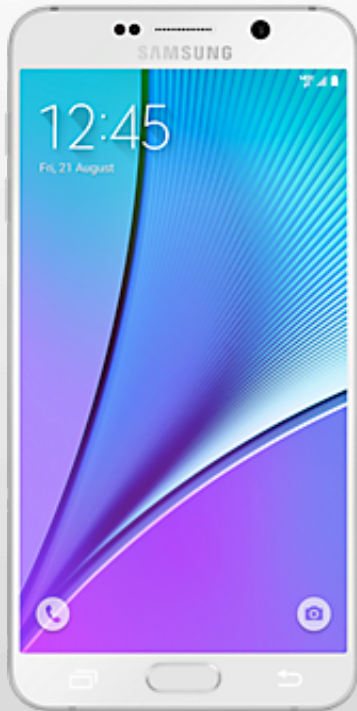
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## HPC Concepts

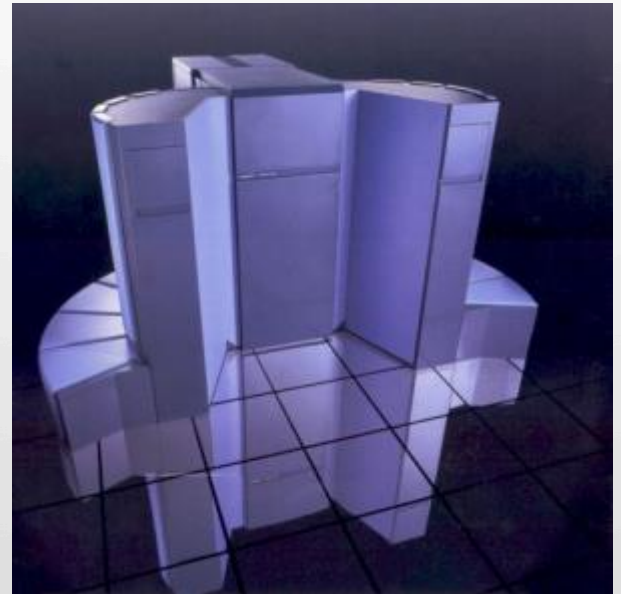
# Supercomputers become history quickly!

Smartphone - 2015



<b>\$740</b>	Cost	<b>\$20,000,000</b>
<b>4 GB</b>	Memory	<b>128 MB</b>
<b>64 GB</b>	Storage	<b>30 GB</b>
<b>302 GFLOPS</b>	Speed	<b>2 GFLOPS</b>

Supercomputer - 1989



# Big Numbers

## Prefix

- K
  - kilo,  $10^3$ , thousand
- M
  - mega,  $10^6$ , million
- G
  - giga,  $10^9$ , billion
- T
  - tera,  $10^{12}$ , trillion
- P
  - peta,  $10^{15}$ , quadrillion
- E
  - exa,  $10^{18}$ , quintillion

## Example: bytes

- 1KB – very small
- 12MB L2 cache per core
- 48GB memory per node
- .5 TB disk space per user
- 4 PB aggregate storage
- Exascale systems – current research area



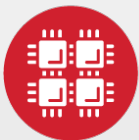


# HPC Terminology

- Cluster
  - A group of computers (nodes) connected by a high-speed network, forming a supercomputer
- Node
  - Equivalent to a high-end workstation, part of a cluster
- Core
  - A processor (CPU), multiple cores per processor chip
- FLOPS
  - “FLoating-point Operations (calculations) Per Second”





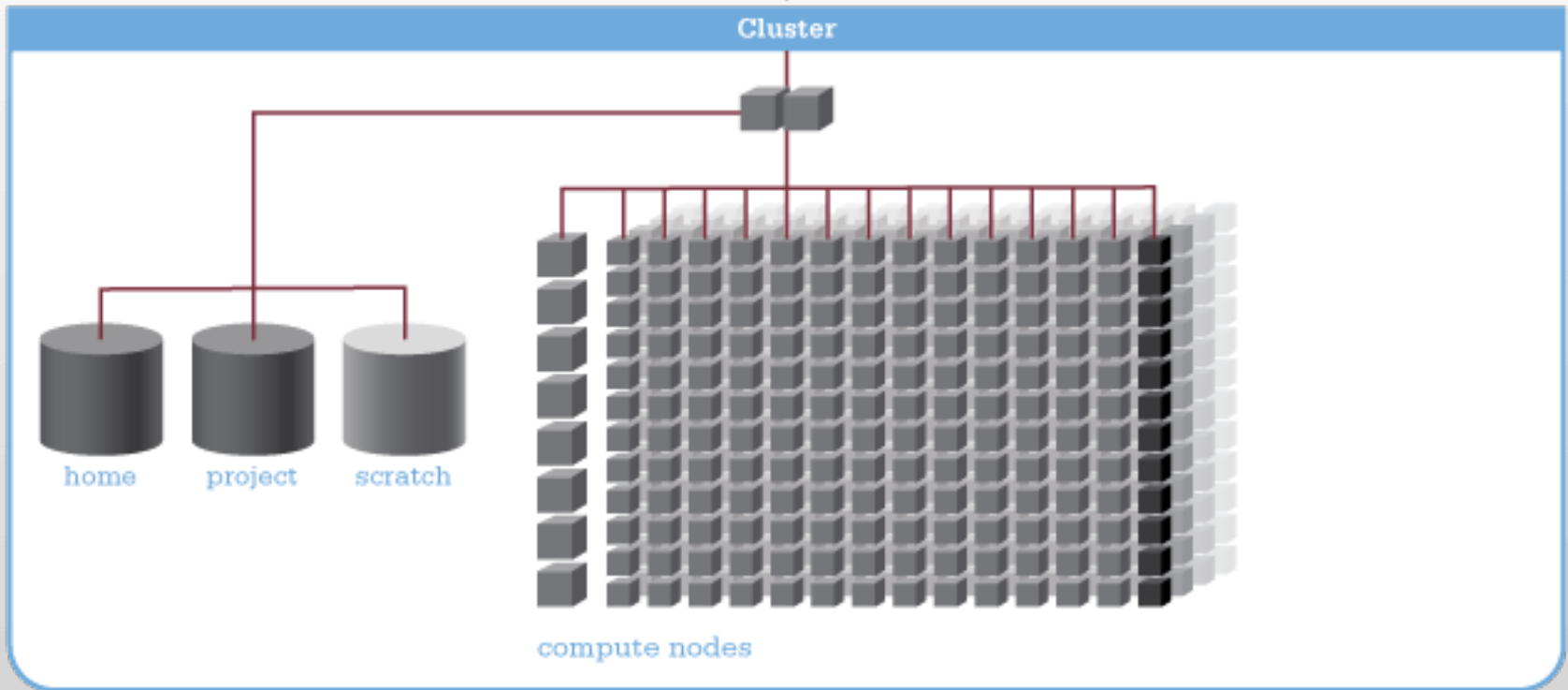
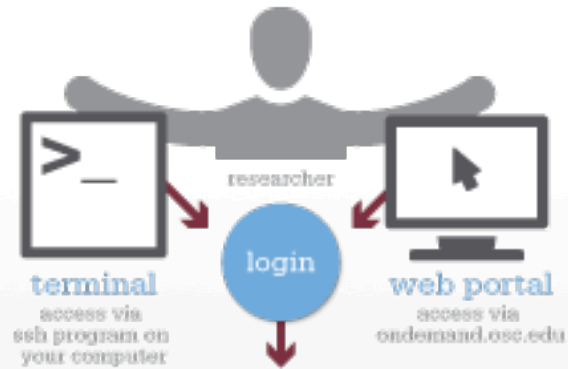


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## Hardware Overview

# Organization of a Supercomputer





# Login Nodes – Usage

- Purpose
  - Submit jobs to batch system
  - Edit files
  - Manage your files
  - Interactive work – small scale
- Limits
  - 20 minutes CPU time
  - 1GB memory
- Use the batch system for serious computing!



# Supercomputers at OSC

- Ruby cluster (small cluster, limited access)
  - Online March 2015
  - Named for Ruby Dee, actress, poet, playwright, screenwriter, journalist and activist. She was born in Cleveland.
  - HP system, Intel Xeon processors, 4800 cores
- Oakley cluster
  - Online March 2012
  - Named for Annie Oakley, famous Ohio sharpshooter
  - HP system, Intel Xeon processors, 8280 cores
- Glenn cluster
  - “Glenn phase II” online July 2009 – **retired March 2016**
  - Named for John Glenn, Ohio astronaut and senator
  - IBM 1350, AMD Opteron processors, 3500 cores



# Oakley Cluster



# Login Nodes – Configuration

- Oakley
  - 2 general-purpose login nodes
  - 12 cores, 124 GB memory each
  - Connect to oakley.osc.edu
- Ruby
  - 2 general-purpose login nodes
  - 16 cores, 132 GB memory each
  - Connect to ruby.osc.edu
- Glenn
  - 2 general-purpose login nodes
  - 16 cores, 64 GB memory each
  - Connect to glenn.osc.edu



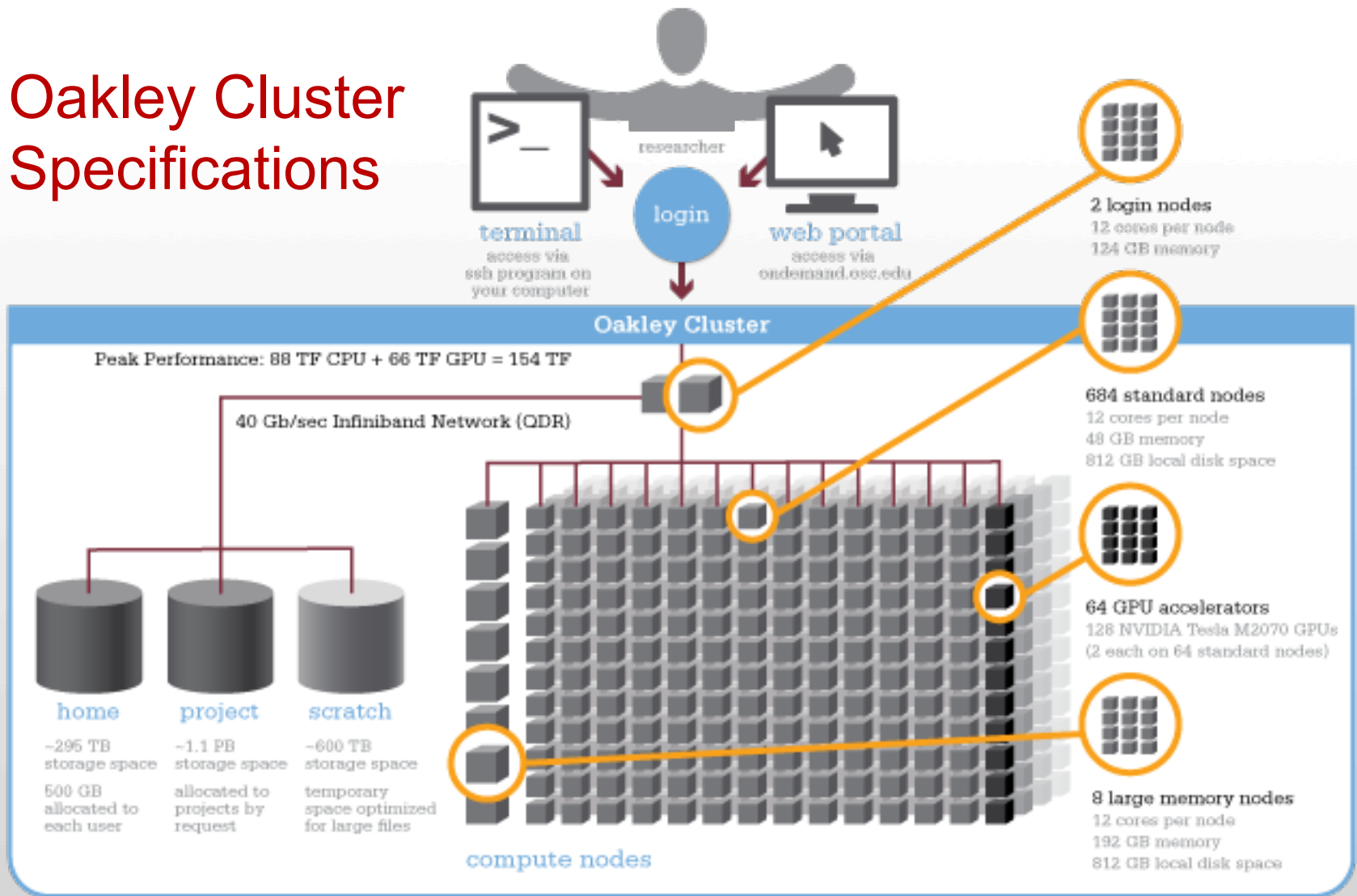
# Compute Nodes – Oakley

- 684 standard nodes
  - 12 cores per node
  - 48 GB memory (4GB/core)
  - 812 GB local disk space
- 8 large memory nodes
  - 12 cores per node
  - 192 GB memory (16GB/core)
  - 812 GB local disk space
- Network
  - Nodes connected by 40Gbit/sec Infiniband network (QDR)





# Oakley Cluster Specifications





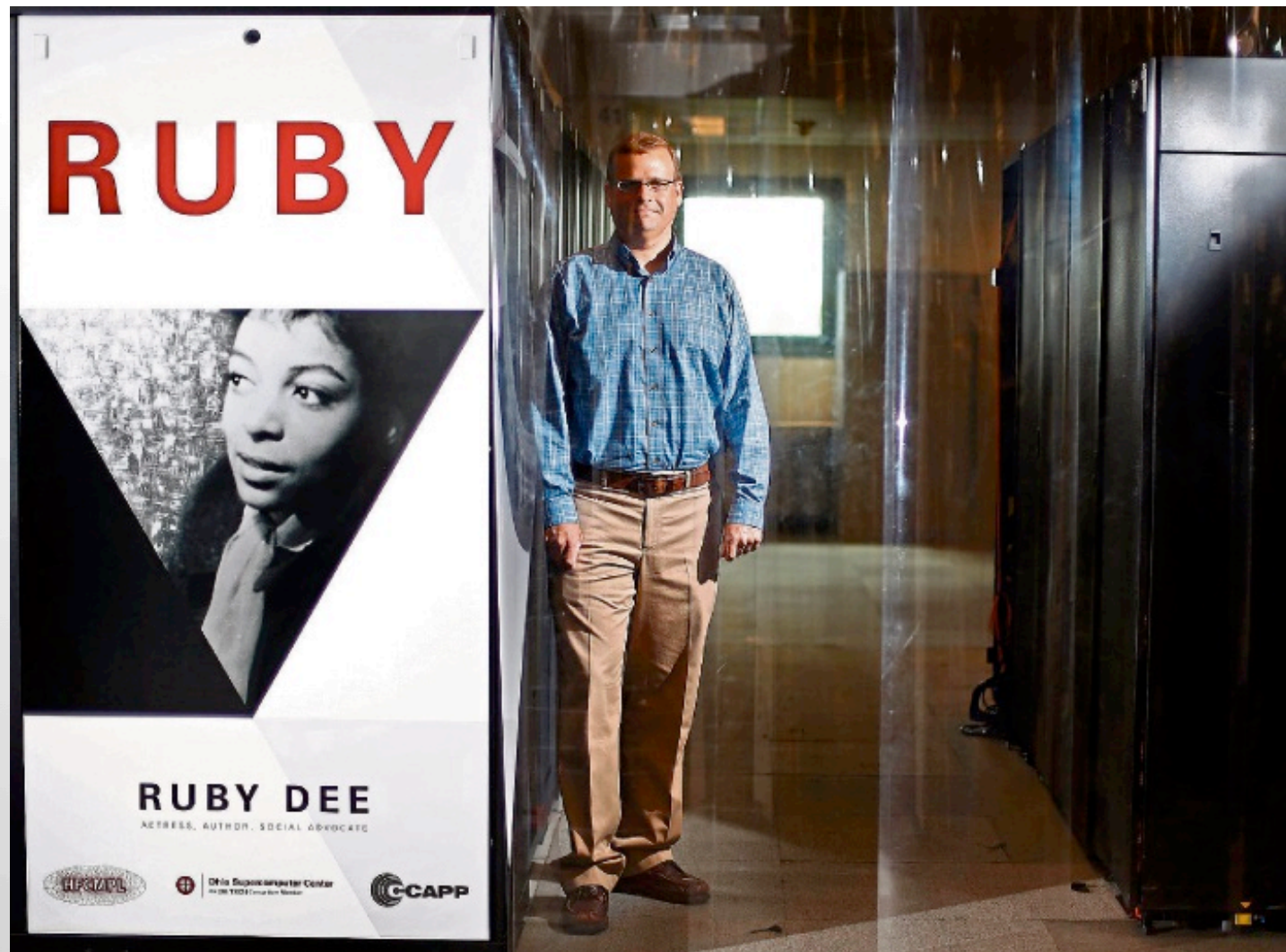
# Specs: Oakley Cluster vs. Top 500 Systems in the World



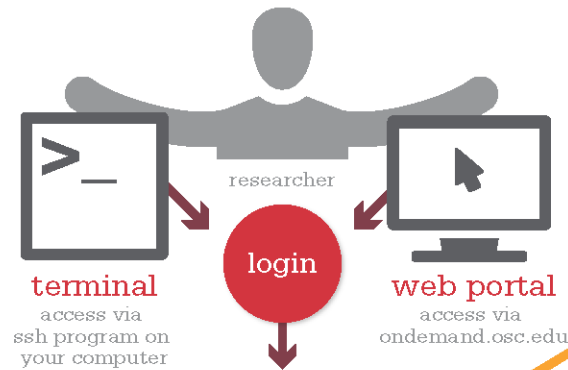
Metric	June 2012	June 2012	November 2012	November 2012	June 2013
	Performance Ranking	Efficiency Ranking	Performance Ranking	Efficiency Ranking	Ranking
Overall Ranking in the World	180 <sup>th</sup>	37 <sup>th</sup>	460 <sup>th</sup>	30 <sup>th</sup>	Not Listed
Overall Ranking in US	89 <sup>th</sup>	8 <sup>th</sup>	235 <sup>th</sup>	8 <sup>th</sup>	Not Listed
Overall Academic Ranking in the World	40 <sup>th</sup>	9 <sup>th</sup>	91 <sup>st</sup>	13 <sup>th</sup>	Not Listed
Overall Academic Ranking in US	11 <sup>th</sup>	2 <sup>nd</sup>	23 <sup>rd</sup>	2 <sup>nd</sup>	Not Listed



# OSC's Newest HPC System: Ruby Cluster



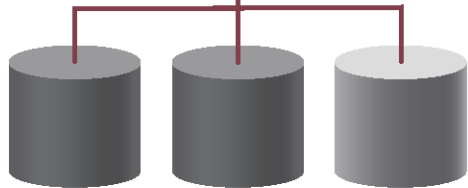
# Ruby Cluster Specifications



## Ruby Cluster

Peak Performance: 96 TF CPU + 48 TF Accelerator = 144 TF

56 Gb/sec Infiniband Network (FDR/EN)



home

~295 TB  
storage space

500 GB  
allocated to  
each user

project

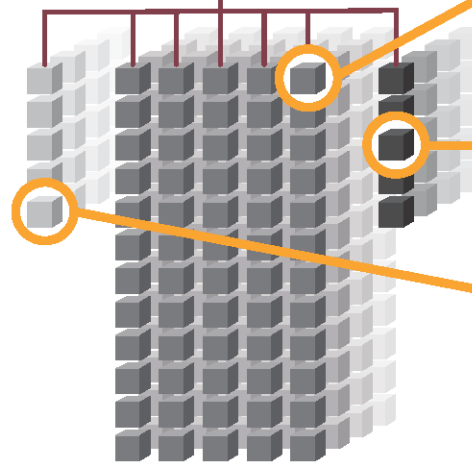
~1.1 PB  
storage space

allocated to  
projects by  
request

scratch

~600 TB  
storage space

temporary  
space optimized  
for large files



compute nodes



2 login nodes

16 cores per node  
132 GB memory



240 standard nodes

Intel Xeon E5 2670 V2  
(Ivy Bridge) CPUs  
20 cores per node  
64 GB memory  
1 TB local disk space



22 NVIDIA Tesla GPUs

1 each on 20 standard nodes  
2 on the debug node



20 Intel Xeon Phi  
Coprocessors

1 each on 20 standard nodes



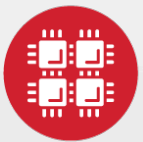
# OSC File Space Information

- Scratch - Lustre – Parallel File System ~570 TBs (all disk)
- Project - GPFS
  - ~1.1PB total usable (Disk)
  - Hierarchical storage capable to tape subsystem
  - Allocated to projects in TBs, for limited time periods
- Home Directory Space / NFS
  - ~295 TBs usable (Disk)
  - Allocated to each user, 500 GB quota limit

## Mass Storage Overview

- 2 Petabytes (PBs) of usable disk
- 1100 TBs GPFS storage
- 570 TBs Lustre storage
- 1.8 PBs tape





# Ohio Supercomputer Center

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## Resource Grants and Accounts at OSC



# Who can get an account?

- Academic accounts
  - 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 accounts are also available
  - No cost to Ohio academic users
- Commercial accounts
  - Commercial organizations may purchase time on OSC systems





# Accounts and Projects at OSC

- Project
  - Headed by a PI
  - May include other users
  - Basis for accounting at OSC
  - Submit proposal for computing resources for a project
- Account
  - Username and password to access HPC systems
  - Each account associated with one project
  - Each account used by one person (please!)
  - If you work on multiple projects, you will have multiple accounts.





# Allocations and Charges

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





# Getting an Account

- 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)
- Condo model for HPC





## Citing OSC

- Please cite OSC in your publications:
  - Details at [www.osc.edu/citation](http://www.osc.edu/citation)
- These publications should be reported to OSC





# ARMSTRONG Researcher Portal

- <https://armstrong.osc.edu>
- Manage your project and accounts
  - Monitor resource utilization on all your projects
  - Add authorized users (request accounts) – PIs only
- View current information
  - OSC system notices
  - Research opportunities
- Post publications



# ARMSTRONG Researcher Portal

<https://armstrong.osc.edu>

The screenshot displays the user interface of the ARMSTRONG Researcher Portal. At the top, the browser address bar shows the URL <http://ohiosuperusers.ning.com/profile/IanMacConnell>. The page header includes the Ohio Supercomputer Center logo and navigation tabs such as 'Main', 'Invite', 'My Page', 'Members', 'Forum', 'Events', 'Groups', 'Blogs', 'Notes', 'FAQ', 'Chat', 'My Storage', and 'Manage'.

The main content area is titled 'Welcome, Ian MacConnell!' and features a profile picture of Ian MacConnell holding a fish. Below the photo are several management options: 'Manage My Page or Photo', 'Manage My Profile', 'Select A Project', 'Request Resource Units', and 'Manage OSC Accounts'. A status indicator shows '1357/5000 Units Remaining'.

A central bar chart displays 'Resource Unit Utilization over the last 30 Days'. The chart shows daily usage with a peak around day 14. The x-axis is labeled with dates from 01 to 30, and the y-axis ranges from 0e-06 to 2e-05. Below the chart, statistics are provided: Minimum/day: 0.0000, Average/day: 0.0000, Maximum/day: 0.0000, and Total RUs over time period: 0.0000.

Below the chart is a 'My Publications' section with an 'Add Publications' button. The list includes:

1. Kelley, H, MacConnell, I, and Abel: "An Analysis of Identity Links on the ARMSTRONG Portal". Next Steps, Wood, D, Decker, S, and MacConnell, I (Eds.), Columbus, OH (2010). [An online version is also available for download.](#)
2. Berrueta, D, Labra, JE, and MacConnell, I: "XSLT+SPARQL : Scripting the ARMSTRONG Portal with SPARQL embedded into XSLT stylesheets". In: 4th Workshop on Scripting for the ARMSTRONG Portal, Bizer, C, Auer, S, Grimmes, GA, and Heath, T (Eds.). Tenerife (2008). [An online version is also available for download.](#)

On the right side of the page, there is a sidebar with user options: 'Sign Out', 'Inbox', 'Alerts', 'Friends - Invite', and 'Settings'. Below this is an 'Events' section listing 'The X10 Language and Tools for Advanced HPC Programming Workshop' on August 10, 2010. Further down is an 'OSC News & Info' section with 'OSC Supercomputing System Notices' and 'OSC's Calendar of Events'.





# MyOSC

- Site for managing your identity at OSC
- Update your email
- Change your password
- Recover access to your account
- Change your shell
- And a lot more in the future
  - Project reporting
  - Authorized user management
  - Requesting services (e.g. software access)





## Your Contact Info

- Keep your contact information current
  - Use [my.osc.edu](http://my.osc.edu) to manage your account details.
- If your student continues to use OSC after graduation, make sure email address is updated
  - Acceptable if still collaborating with you
- May need to contact you about problems
- Will need to contact you about regular password changes
- You can opt out of routine notifications



# Connecting to the Oakley or Ruby Cluster

- Connect to OSC machines using `ssh` (secure shell)
  - From a Linux/UNIX machine : At prompt, enter  
`ssh userid@oakley.osc.edu`  
`ssh userid@ruby.osc.edu`
  - From a Mac: Enter `ssh` command in TERMINAL window
  - From Windows: `ssh` client software needed
    - Both commercial and free versions are available
- New: Connect using OnDemand portal (web-based)



# OSC OnDemand

- 1: User Interface
  - Web based
    - Usable from computers, tablets, smartphones
    - Zero installation
  - Single point of entry
    - User needs three things
      - [ondemand.osc.edu](http://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 (Abaqus, Ansys, Comsol, Paraview)
  - Terminal Access

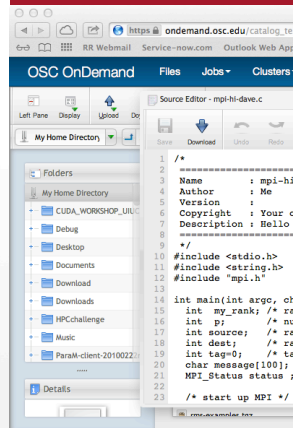




# File Transfer & Editing

# Visualization

## Common Catalog



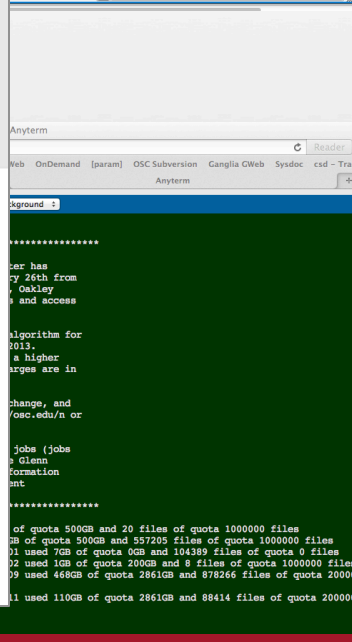
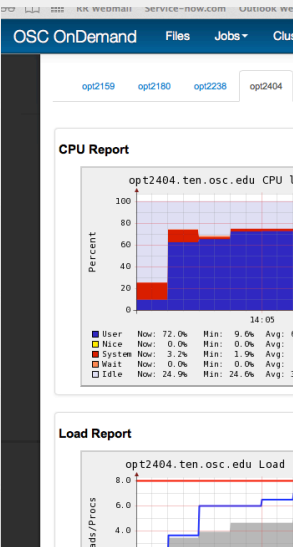
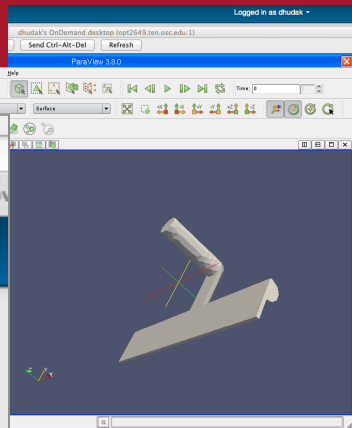
where you go to do everything at OSC

OSC OnDemand provides an integrated, single access point for all of your resources on Glenn and Oakley.

**OSC OnDemand**

where you go to do everything at OSC

OnDemand provides an integrated, single access point for all of your resources on Glenn and Oakley.



# Job Submission & Monitoring

# Command Line



**Ohio Supercomputer Center**

**OH-TECH** | Ohio Technology Consortium  
A Division of the Ohio Board of Regents

# System Status

- Check system status on:
  - <https://www.osc.edu/supercomputing> (bottom of page)
  - Message of the day (/etc/motd) – displayed at login
  - Twitter: @HPCnotices
  - Email for major outages or problems
- Scheduled downtimes
  - Quarterly maintenance – one day outage
  - Jobs held for up to two weeks prior





# 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
  - Headed by a chairperson elected yearly
- Standing committees
  - Allocations
  - Software and Activities
  - Hardware and Operations
- Get involved!
  - Next meeting is October in Columbus



# Demo

- Website tour: [www.osc.edu](http://www.osc.edu)
- ARMSTRONG: <https://armstrong.osc.edu>
- MyOSC: <https://my.osc.edu/>

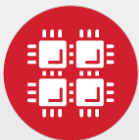




# Demo

- Website tour: [www.osc.edu](http://www.osc.edu)
- MyOSC: <https://my.osc.edu/>
- OnDemand [ondemand.osc.edu](http://ondemand.osc.edu)





# Ohio Supercomputer Center

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## What's New at OSC

# C16 – available Oct. 1<sup>st</sup> (partial Aug. 1<sup>st</sup>)

## Compute Nodes

- 648 standard nodes
  - 28 cores per node (2 14-core Intel Xeon processors)
  - 128 GB memory
  - 1 TB local disk space
- 160 GPU Ready nodes
  - Waiting for NVIDIA's next generation Pascal GPUs
- Network
  - Nodes connected by 100Gbit/sec Infiniband network (EDR)





# C16 – available Oct. 1<sup>st</sup> (partial Aug. 1<sup>st</sup>)

## Special Resources

- 8 large memory nodes
  - 48 cores per node
  - 1536 GB memory (32GB/core)
  - 1 TB local disk space
- 8 large memory/large disk nodes
  - 48 cores per node
  - 1536 GB memory (32GB/core)
  - 48 TB local disk space





# System Configurations

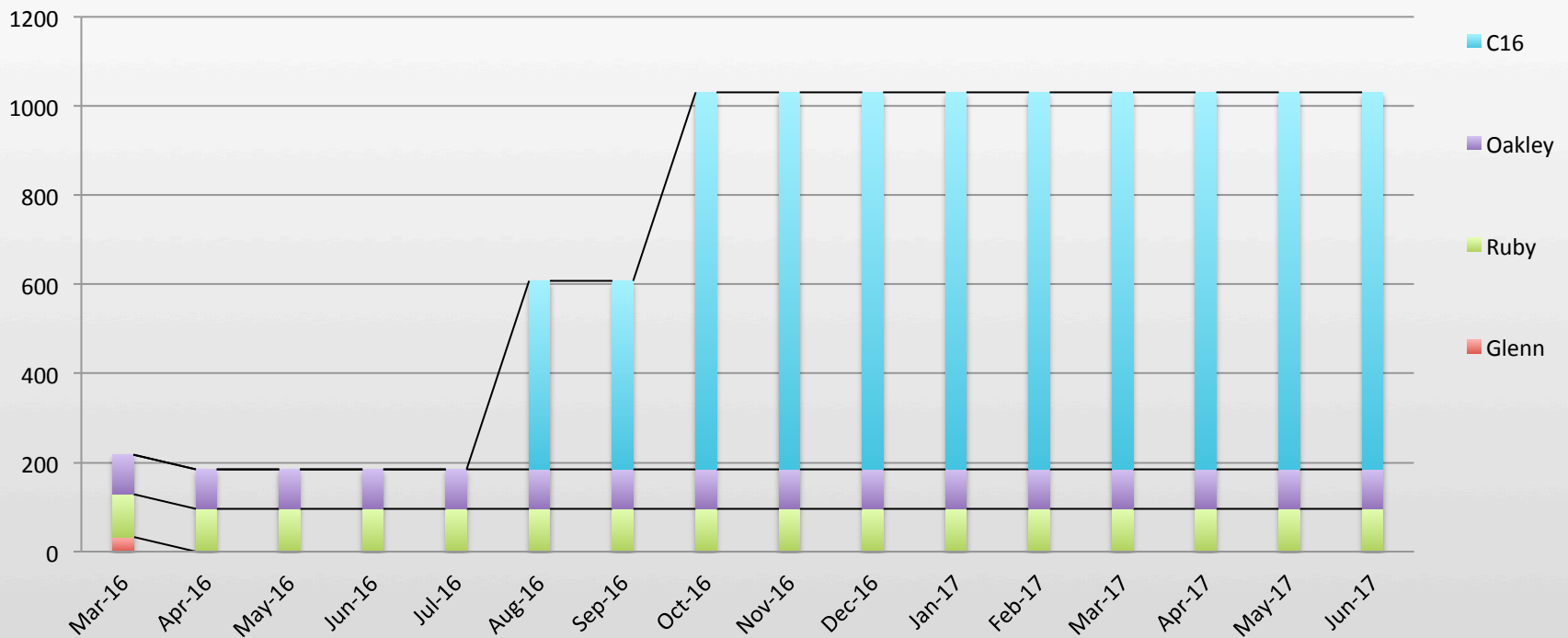
	C16 (2016)	Ruby (2014)	Oakley (2012)
Theoretical Performance	~750 TF	~144 TF	~154 TF
# Nodes	~820	240	692
# CPU Cores	~23,500	4800	8304
Total Memory	~120 TB	~15.3 TB	~33.4 TB
Memory per Core	>5 GB	3.2 GB	4 GB
Interconnect	EDR IB	FDR/EN IB	QDR IB



# C16 – available Oct. 1<sup>st</sup> (partial Aug. 1<sup>st</sup>)

## Performance Increase

Peak Performance



# OSC File Space Information Update

- Scratch – DDN GPFS
  - 1 PB (~570 TB today)
  - 40-50 GB/s peak performance (~10 GB/s today)
- Project – DDN GPFS
  - 3.4 PB usable space (~1.1 PB today)
  - 40-50 GB/s peak performance (8-9 GB/s today)
- **Expected June/July**
- Home Directory Space / (Net App) NFS
  - **New system online in May**
  - ~900 TB usable (Disk) (~300 TB today)
  - Allocated to each user, 500 GB quota limit

## Mass Storage Update

- >5 Petabytes (PBs) of usable disk
- 3.4 PB Project storage
- 1 PB Scratch space available
- 1.8 PBs tape – will be expanded



# Questions

**Kate Cahill**

Education & Training Specialist

Ohio Supercomputer Center

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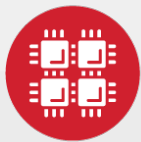


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# Ohio Supercomputer Center

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## User Environment



# Linux Operating System

- “UNIX-like”
- Widely used in HPC
- Mostly command-line
- Choice of shells (bash is default)
- Freely distributable, open-source software
- Tutorials available
- [www.linux.org](http://www.linux.org)



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  - From Windows: `ssh` client software needed
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    - Usable from computers, tablets, smartphones
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  - Single point of entry
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      - OSC Username
      - OSC Password
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  - Job Management
  - Visualization Apps
    - Desktop access
    - Single-click apps (Abaqus, Ansys, Comsol, Paraview)
  - Terminal Access

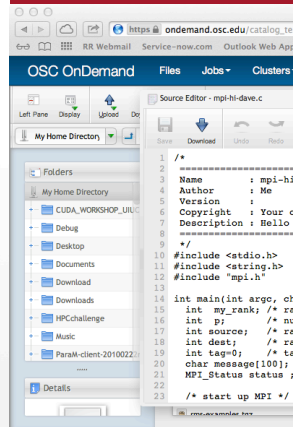




# File Transfer & Editing

# Visualization

## Common Catalog

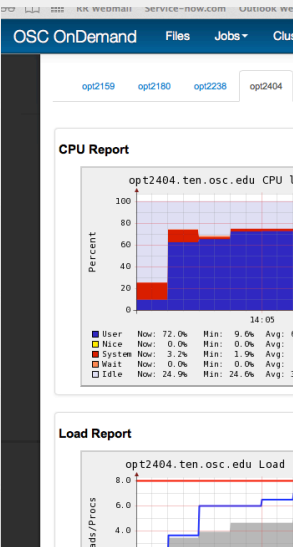
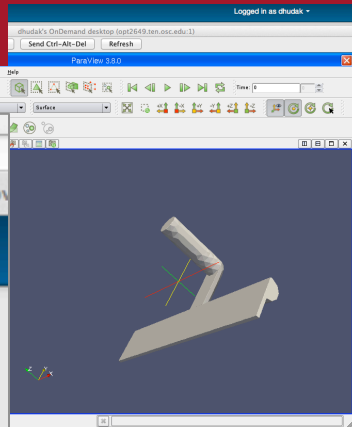


OSC OnDemand Files Jobs Clusters Apps Help

# OSC OnDemand

where you go to do everything at OSC

OnDemand provides an integrated, single access point for all of your resources on Glenn and Oakley.



```

Anyterm
Web OnDemand [param] OSC Subversion Ganglia OWeb Sysdoc csd - Trac
Anyterm
background :
*****
User has
by 26th From
Oakley
and access
algorithm for
2013.
a higher
arges are in
change, and
/osc.edu/n or
jobs (jobs
Glenn
formation
ent
*****
of quota 500GB and 20 files of quota 1000000 files
38 of quota 500GB and 557205 files of quota 1000000 files
31 used 1GB of quota 200GB and 104319 files of quota 0 files
02 used 1GB of quota 200GB and 8 files of quota 1000000 files
09 used 468GB of quota 2861GB and 878266 files of quota 200000
11 used 110GB of quota 2861GB and 88414 files of quota 200000
  
```

# Job Submission & Monitoring

# Command Line



# Connecting to an OSC Cluster with Graphics

- Programs on the cluster can have an X-based GUI
  - Display graphics on your computer
- Linux/UNIX and Mac: Use `-X` flag
  - `ssh -X userid@oakley.osc.edu`**
- Windows: Need extra software
  - Both commercial and free versions are available
  - Configure your ssh client to tunnel or forward X11
- Primarily used with programs on login node
  - Can also use with interactive batch jobs



# Transferring Files to and from the Cluster

- Most file transfers to and from OSC machines use `sftp` or `scp`
  - Linux and Mac have them built in
  - Windows needs extra software
- For small files, connect to login node  
`oakley.osc.edu`
- For large files, transfer may fail due to shell limits
  - Connect to `gridftp01.osc.edu` (file transfer only)



# Text editing

- Traditional Unix editors
  - `vi`
  - `emacs`
  - Many books and web pages about `vi` and `emacs`
- GUI editor
  - `gedit`
- Simple editor
  - `nano`
- Can also edit on your computer and transfer files back and forth
  - `dos2unix`, `unix2dos`, `mac2unix`





# Demo

- OSC OnDemand
- ssh
- sftp
- Linux
- Home directory tree
- Text editor: nano



## Adding or Removing Software from Your Environment

- Load the module for the software you need, e.g.,
  - `module load comsol`
- Allows multiple versions of software to coexist on our system
- Allow us to make changes without affecting you
  - PLEASE DON'T HARDCODE PATHS!
- Can load modules at command prompt or in your `.bash_profile` or `.bashrc` file
- Also load modules in your job (batch) scripts



# Modules and your shell environment

- How modules work
  - Modify environment variables like `$PATH` and `$MANPATH` within your shell
- Default set of modules loaded at login
  - module system, batch system (do not unload)
  - default compiler and MPI modules
- Do NOT completely replace `$PATH` in your `.bash_profile` or `.bashrc`
- DO prepend directories to the existing `$PATH`
  - Type: `export PATH=$HOME/bin:$PATH`



# Module Commands

- What modules do you have loaded?
  - `module list`
- What modules are available?
  - `module spider` or `module avail`
- Multiple versions of the same software
  - `module avail intel`
- Add a software module to your environment
  - `module load cuda`
- Remove a software package from your environment
  - `module unload intel`
- Load a different software version
  - `module swap intel intel/13.1.3.192`





# File Permissions

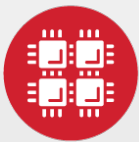
- By default all files are readable by all users
- Check permissions using `ls -l`

```
-rw-r--r-- 1 osu7824 PAS0925 10839 Jan 13 2015 triarm_VVvacid.sdf
-rw-r--r-- 1 osu7824 PAS0925 11667 Jan 13 2015 triarm_VVvester.sdf
drwxr-xr-x 8 osu7824 PAS0925 4096 Jan 16 2014 tutorial
-rw-r-x--- 1 osu7824 PAS0925 9917889 Jan 15 2015 ValBaskEst32_gopt.log
-rw-r--r-- 1 osu7824 PAS0925 12818 Jan 15 2015 ValBaskEst32_gopt.mol2
-rwxr-xr-x 1 osu7824 PAS0925 453376 Feb 26 2015 ValBaskEst_c0_ValBaskEst0-CyHexPO-2OMe-cl1_md1.mdcrd
```

- `-rwxr-xr-x` User, Group, Others
- Change file permissions using `chmod`  
`chmod u=rw,g=r file`

```
chmod -R u=rw,g=r directory
```





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## Storage



# Home Directories

- Each user has a home directory
- Visible from all OSC systems
- Backed up daily – “permanent storage”
- Quotas
  - 500GB of storage per user account
  - 1,000,000 files maximum
  - Cannot create new files if over quota
  - Quota and usage info displayed at login



# Project Directories

- PI may request project directory if more space needed
  - Send request to OSC Help
  - Large requests are reviewed by SUG Allocations Committee
  - Shared by all users in the project
- Backed up daily
- Visible from all OSC systems
- Project quota is separate from the home directory quota



# Sample Quota Display

Quota display at login (information collected nightly):

```
As of 2010 Jul 15 04:02 userid usr1234 on /nfs/06 used 28GB of
quota 500GB and 41374 files of quota 1000000 files
As of 2010 Jul 16 04:02 project/group PRJ0321 on /nfs/proj01
used 27GB of quota 5000GB and 573105 files of quota 1000000
files
```

Output from `quota` command (run manually):

```
Disk quotas for user usr1234 (uid 11059):
```

```
Filesystem
```

	blocks	quota	limit	grace	files	quota	limit	grace
fs06-oak.ten.osc.edu:/nfs/06/osc	201698292	450000000	524288000		631137	950000	1000000	





# File Management

- Compress large, rarely used files
  - Use `gzip` or `bzip2` commands
- Combine large numbers of small files into an archive
  - Use `tar` command



# Parallel File System – Lustre

- Designed to handle heavy parallel I/O load
- Faster access than home and project directories
- NOT good for small files
- Visible from all cluster nodes (shared)
- Suitable for short-term storage (up to 6 months) of large amounts of data
- Also useful as batch-managed temporary storage
- **Scratch storage – NOT backed up!**



## Local Disk – \$TMPDIR

- Local file system on each compute node
  - 812 GB on each Oakley node
  - 1 TB on each Ruby node
- Fast – use for intermediate or scratch files
- Not shared between nodes
- Not backed up
- Managed by the batch system
- Data removed when job exits

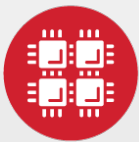




# Overloading the File Servers

- “*A supercomputer is a device for turning compute-bound problems into I/O-bound problems.*” --Ken Batcher (parallel computing pioneer)
- One user’s heavy I/O load can affect responsiveness for all users on that file system
- **Never** do heavy I/O in your home or project directory!
- Use \$TMPDIR, copying files in and out as necessary
- Don’t let large numbers of jobs run in lockstep.



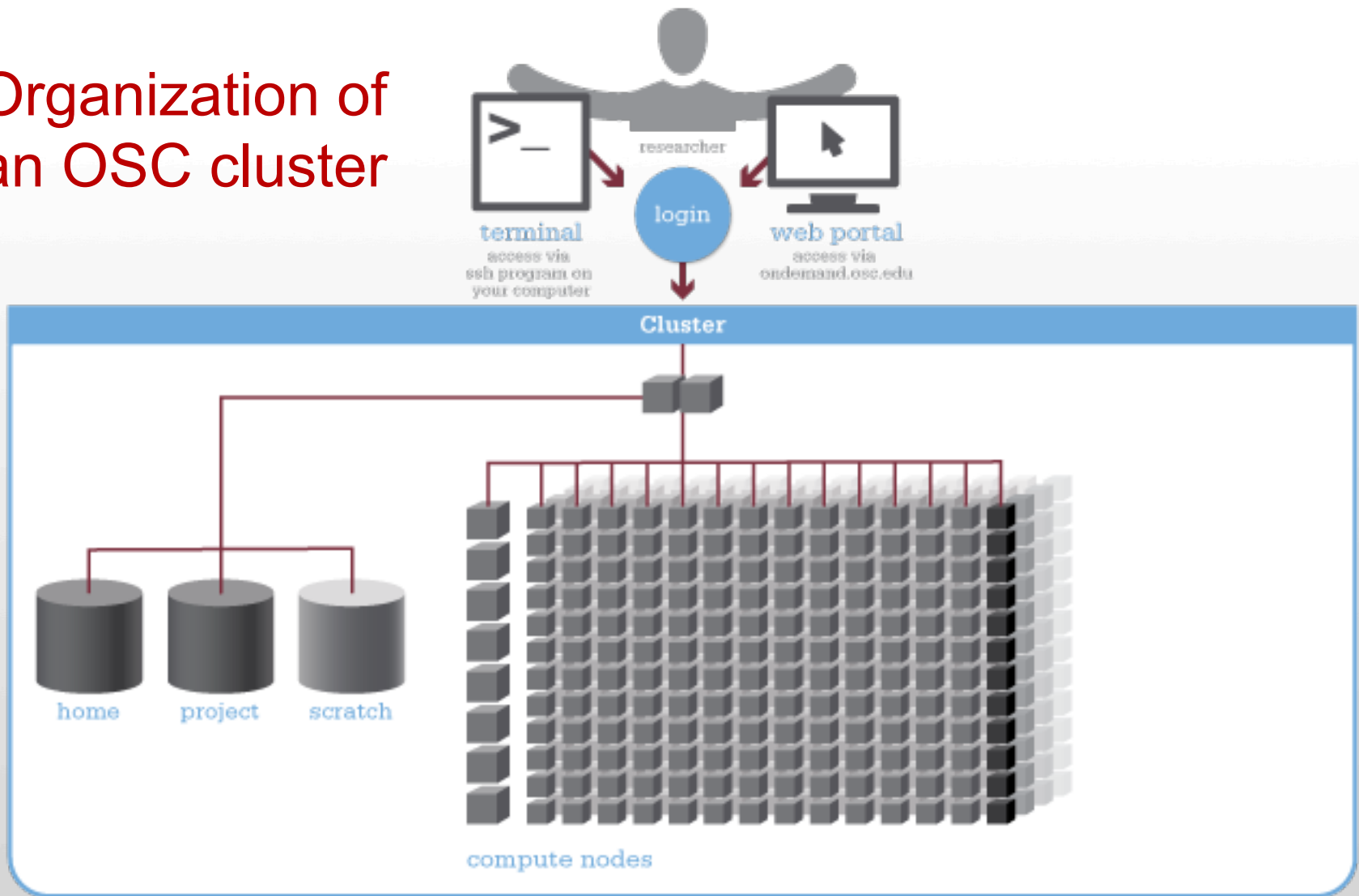


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## Batch Processing

# Organization of an OSC cluster

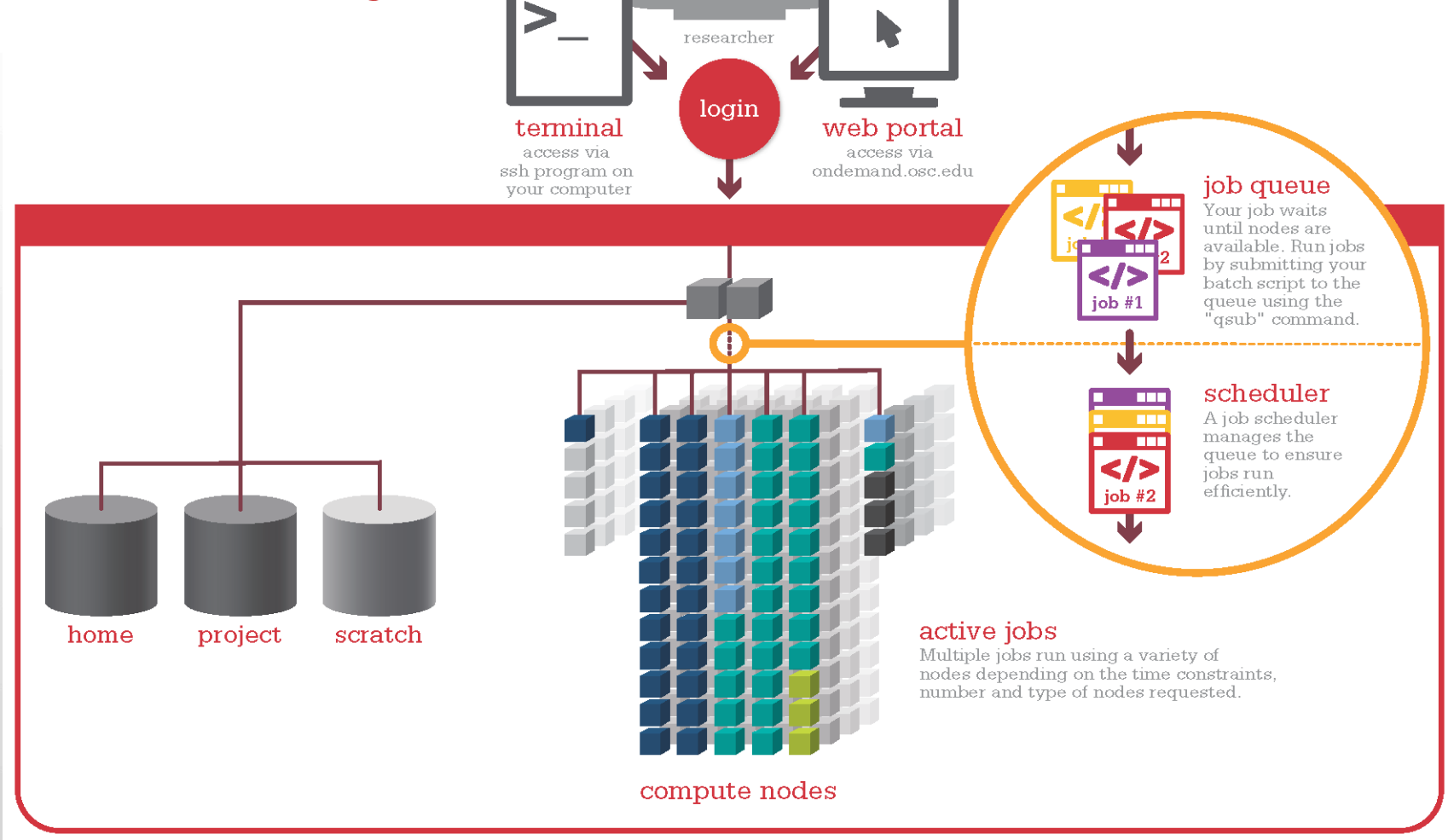


# Batch System at OSC

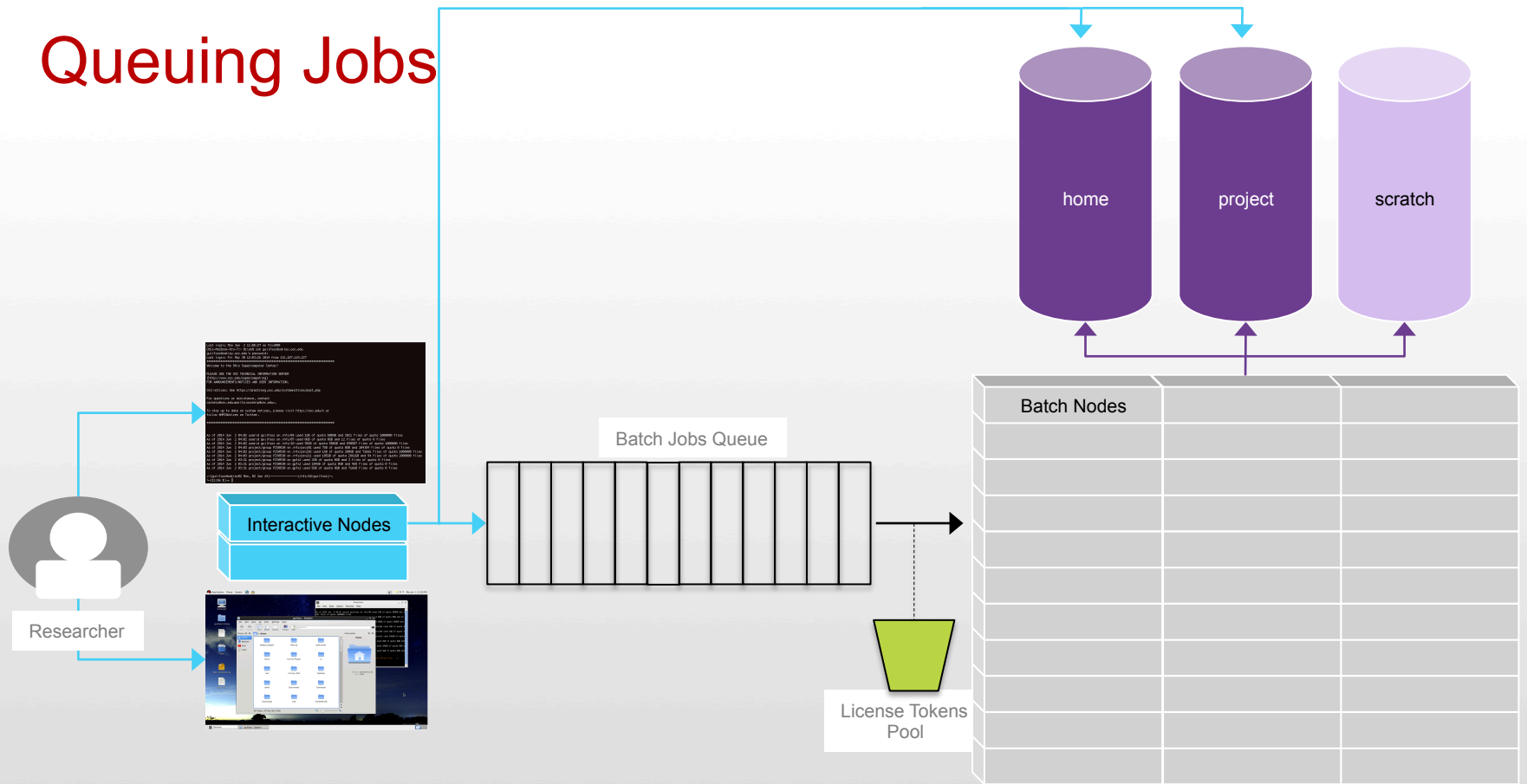
- Compute nodes are allocated through the batch system
  - PBS – Portable Batch System
  - Torque – resource manager
  - Moab – scheduler
- Documentation at [www.osc.edu/supercomputing/batch-processing-at-osc](http://www.osc.edu/supercomputing/batch-processing-at-osc)



# Why do supercomputers use queueing?



# Queuing Jobs



Run jobs by submitting your batch script to the compute nodes using the "qsub" command.

Your job is submitted to a queue and will wait in line until nodes are available. Queues are managed by a job scheduler that allows jobs to run efficiently.





## Idea Behind Batch Processing

- Whatever you would normally type at the command prompt goes into your batch script
- Output that would normally go to the screen goes into a log file (or files)
- The system runs your job when resources become available
- Very efficient in terms of resource utilization





# Running a Job on the Compute Nodes

- Create a batch script for a job
- Submit the job
- Job gets queued
- Job runs when resources become available
- Get your results when the job finishes





# Specifying Resources in a Job Script

- Nodes and cores (processors) per node
- Memory
- GPUs
  - See “Batch Processing at OSC” on OSC website
- Walltime
  - Overestimate slightly – job will be deleted if it hits limit
  - Shorter job may start sooner due to backfill
- Software licenses
  - See specific software page on OSC website



# Sample Batch Script

```
#PBS -N serial_fluent
#PBS -l walltime=1:00:00
#PBS -l nodes=1:ppn=1
#PBS -j oe
#PBS -l software=fluent+1
# Set up the FLUENT environment
module load fluent
# Move to directory job was submitted from
cd $PBS_O_WORKDIR
# Copy input files to compute node
cp run.input $TMPDIR
cd $TMPDIR
# Run fluent and copy results back to home
fluent 3d -g < run.input
cp `results*` $PBS_O_WORKDIR
```

Job setup information  
for PBS

# This is a comment

Commands  
to be run

Put all this into a text file!



# Submitting a Job and Checking Status

- Command to submit a job
  - `qsub script_file`
- Response from PBS (example)
  - `123456.oak-batch.osc.edu`
- Show status of batch jobs
  - `qstat -a jobid`
  - `qstat -u username`
  - `qstat -f jobid`



# Scheduling Policies and Limits

- Walltime limit
  - 168 hours for serial jobs (single node)
  - 96 hours for parallel jobs (multiple nodes)
- Per-user limits
  - 128 concurrently running jobs
  - 2040 processor cores in use
  - 1000 jobs in the batch system, running or queued
- Per-group limits
  - 192 concurrently running jobs
  - 2040 processor cores in use





# Waiting for Your Job To Run

- Queue wait time depends on many factors
  - System load
  - Resources requested
    - nodes, cores, large memory, gpus, software licenses
  - Fair share limits (if load is high)
    - reduced priority for users or groups using a lot of resources



# Job Output

- Screen output ends up in file *job\_name.ojobid*
  - Copied to your working directory when job ends
  - Example: `testjob.o1234567`
- To see screen output while job is running
  - `qpeek jobid`
  - Example: `qpeek 1234567`



## Interactive Batch Jobs

- Interactive, but handled through batch system
  - Resource limits same as standard batch limits
- Useful for tasks forbidden on login nodes
  - Debug parallel programs
  - Run a GUI program that's too large for login node
- May not be practical when system load is high
  - Long wait, same as standard batch job
- To submit an interactive batch job (example)
  - `qsub -I -X -l nodes=2:ppn=12 -l walltime=1:00:00`





## Batch Queues

- Oakley and Ruby have separate batch systems
  - Submit job and check status on the same cluster
- Debug reservation
  - A few nodes on each system are reserved for short jobs ( $\leq$  1 hour)
  - Special flag required on Ruby: `-q debug`







# Parallel Computing

- Each processor is fast, but real speed comes from using multiple processors
- Multithreading
  - Use multiple cores on a single node
  - Shared memory
- Message passing (MPI)
  - Use one or multiple nodes
  - Distributed memory





## To Take Advantage of Parallel Computing

- Program must be written to take advantage of multiple cores and/or multiple nodes
- Many commercial applications have multithreaded or parallel versions
- Must use `mpirexec` for multiple nodes
- **Can't just request more nodes or cores and expect your job to run faster**

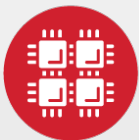


# Specifying Resources in a Job Script for GPUs

- Nodes and cores (processors) per node
- Memory
- GPUs
  - See “Batch Processing at OSC” on OSC website

```
#PBS -l walltime=01:00:00
#PBS -l nodes=1:ppn=1:gpus=1
#PBS -N compute
#PBS -j oe
module load cuda
cd $HOME/cuda
cp mycudaApp $TMPDIR
cd $TMPDIR
./mycudaApp
```





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## Third-Party Software Applications



## Access to Licensed Software

- Most software licenses for academic use only
- Some software requires signed license agreement
  - Check website
  - Contact OSC Help



# Third party applications

- **Chemistry** (\*license agreement required)
  - \*AMBER
  - ChemTools
  - COLUMBUS
  - \*CSD (Cambridge Structural Database)
  - ESPRESSO
  - GAMESS
  - \*Gaussian
  - GROMACS
  - LAMMPS
  - MacroModel®
  - MEAD
  - NAMD
  - NWChem
  - Open Babel
  - \*Turbomole



# Third party applications

- **Bioinformatics**
  - Bioperl
  - BLAST
  - BLAT
  - Bowtie
  - Clustal W
  - EMBOSS
  - Fitmodel
  - HMMER
  - MrBayes
  - NAMD
  - PAML
  - PAUP
  - RAxML
  - RepeatMasker
  - TreeBeST



# Third party applications

- **Structural Mechanics** (\*license agreement required;  
¢ statewide licensed)
  - \*ABAQUS
  - ¢ Altair HyperWorks
  - \*ANSYS
  - COMSOL Multiphysics
  - \*LSDYNA
  - LS-PREPOST







## Third party applications

- **Fluid Dynamics** (\*license agreement required)
  - \*Fluent
  - OpenFOAM



# Third party applications

- Mathematics/Statistics (⌘ statewide licensed)
  - MATLAB (special licensing restrictions)
  - Octave
  - R
  - Stata
  - FFTW
  - ScaLAPACK
  - MINPACK
  - sprng2
  - ⌘ Intel MKL
  - ACML (Glenn only)



# Third party applications

- **General programming software** (⌘ statewide licensed)
  - gnu compilers and debugger
  - ⌘ Intel compilers
  - ⌘ Totalview debugger
  - ⌘ PGI compilers
  - MPI library
  - HDF5
  - NetCDF
  - Java, Java Virtual Machine
  - Python



# Third party applications

- **Parallel programming software** (⌘ statewide licensed)
  - MPI library (mvapich, mvapich2)
  - OpenMP
  - CUDA
  - OpenCL
  - OpenACC





## Third party applications

- **Visualization software**

- GNUplot
- Jmol
- VTK

- More applications can be found at Software page:  
<http://www.osc.edu/supercomputing/software/>

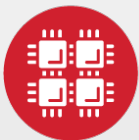




## OSC doesn't have the software you need?

- Commercial 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





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## OSC Policies

Firefox

Supercomputing | Ohio Supercomputer ...

https://www.osc.edu/supercomputing


Home About OSC Supercomputing Cyberinfrastructure Research Education News Contact Us

Home

## Supercomputing

As a leader in high performance computing and networking, the Ohio Supercomputer Center (OSC) is a vital resource for Ohio's scientists and engineers. OSC is a fully-scalable center with mid-range machines to match those found at National Science Foundation centers and other national labs. The Center's flagship supercomputing system is the Oakley Cluster, an 8,300+ core HP Intel Xeon machine.

OSC also is home to the Ohio Interface Labratory, which provides state-of-the-art graphics equipment and output services for computer graphics and animation. Members of the Science and Technology Support Group provide much of the information for this server.



Oakley HP Intel Xeon Cluster (8,328 Cores)

### Getting Started

Welcome to OSC! If you are new to supercomputing, new to OSC, or simply interested in getting an account (if you don't already have one), we have some resources to help you.

- Read about the [basics of High Performance Computing](#) (highly recommended for new users).
- Learn more about [our account allocation process](#), and [how to get started](#).
- Apply for [expanded resources](#) beyond those for a start-up project.
- Get help [connecting to our resources](#).
- Read our [policies](#), [FAQ](#), [code of ethics](#) for users, and [glossary](#).

**OSC Policies**

### Supercomputing

- Getting Started
- HPC Environments
- Available Software
- Portals
- Tutorials & Training
- Support Services
- Search Documentation

### Upcoming Events

August 8, 2013 - [Statewide User Group \(SUG\) General Meeting](#) (Columbus, OH)

August 23, 2013 - [Your Plan For Health Biometric Screenings](#) (Columbus, OH)

September 3, 2013 - [Intro to OSC](#) (Columbus, OH)

[More](#)

### Recent News

*Columbus, Ohio* (July 23, 2013) - [OSC OnDemand gives computational](#)







# OSC Policies

- OSC-1, OSC Data Lifecycle Management Policy
  - Use of home directory, project directory and **\$TMPDIR**
  - Storage and file quotas
  - Backup and recovery





# OSC Policies

- OSC-11, OSC User Management Policy
  - Who can get an account
  - Charges for accounts
  - Types of accounts
  - Account restrictions
  - Account resource units
  - Inappropriate system use



# For More Information

- Key webpages

[www.osc.edu/supercomputing](http://www.osc.edu/supercomputing) - general documentation

<https://www.osc.edu/supercomputing/batch-processing-at-osc>

- Contact the help desk (OSC Help) 24/7

[oschelp@osc.edu](mailto:oschelp@osc.edu)

614-292-1800

1-800-686-6472



# Questions

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# Practice Commands

- In a browser go to *ondemand.osc.edu*
- Use your workshop login info
- Click Clusters, select Oakley Shell Access
  - Might have to enable pop-ups
- Type `module avail` to see available software
- `cp /fs/lustre/kcahill/workshop/new-test.pbs .`
- `nano new-test.pbs`
- `qsub new-test.pbs`
- `qstat -u`
- `qdel`
- `exit`

