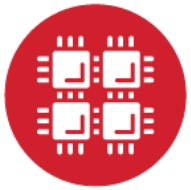

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Computing Services to Accelerate Research and Innovation

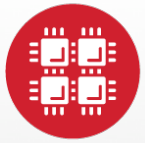
Brian Guilfoos
HPC Client Services Manager

Updated: 9/6/2107

Outline

https://www.osc.edu/

- What is OSC?
- HPC Concepts
- Hardware Overview
- Data Storage Systems
- Batch Processing
- Accessing Available Software
- OnDemand Web Portal Demonstration



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What is the Ohio Supercomputer Center?

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.

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

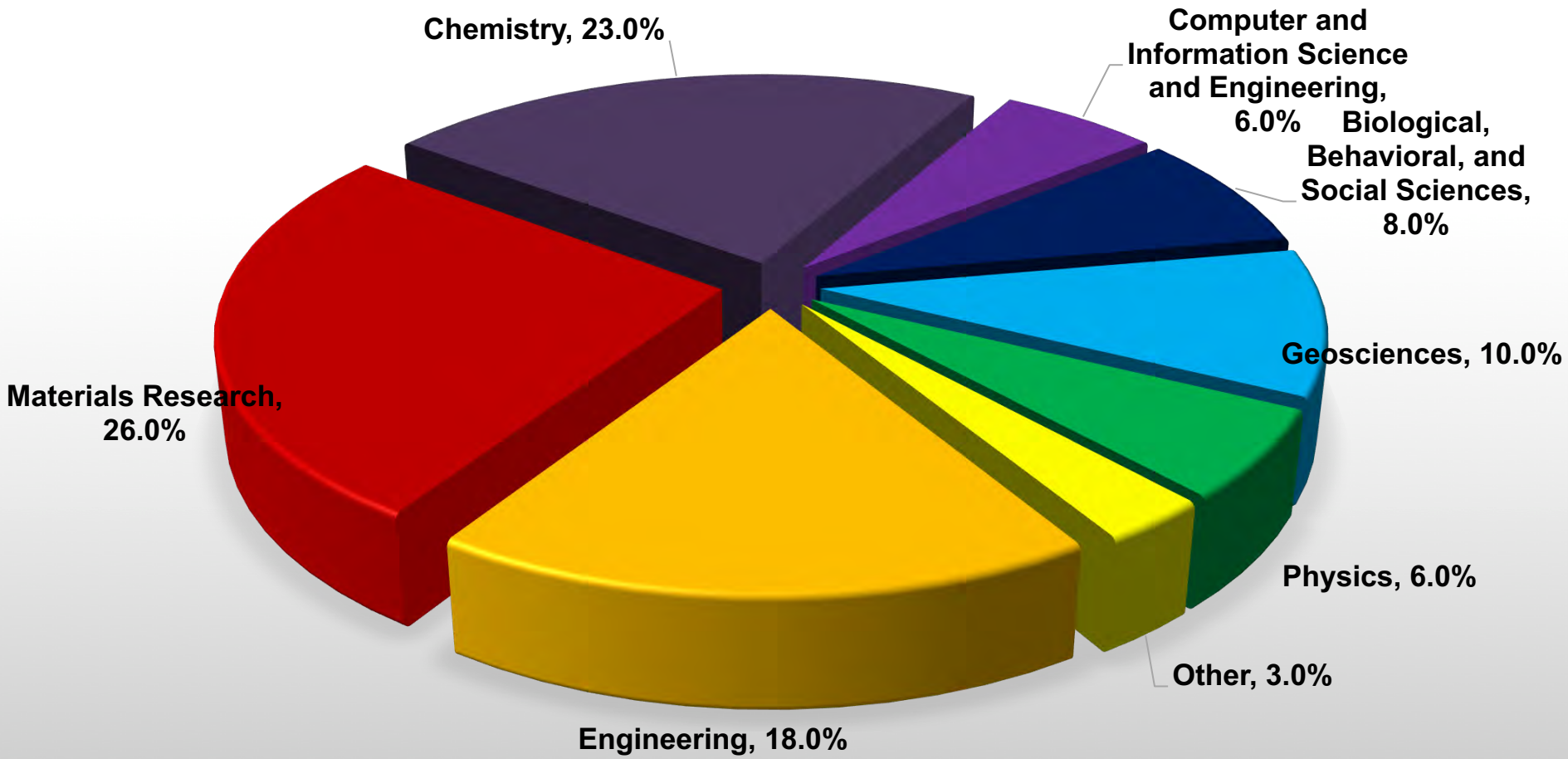
Research & Innovation Center will operate, when opened, as the proving grounds for next-generation technology infrastructure innovations and a catalyst for cutting-edge research and collaboration.

Active Projects
Total: 469

Key

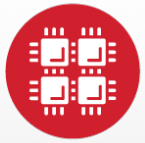
- 1–5
- 6–10
- 11–20
- 21+

Computing Resource Usage by Field of Science (FoS)



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)



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HPC Example Projects & Concepts

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

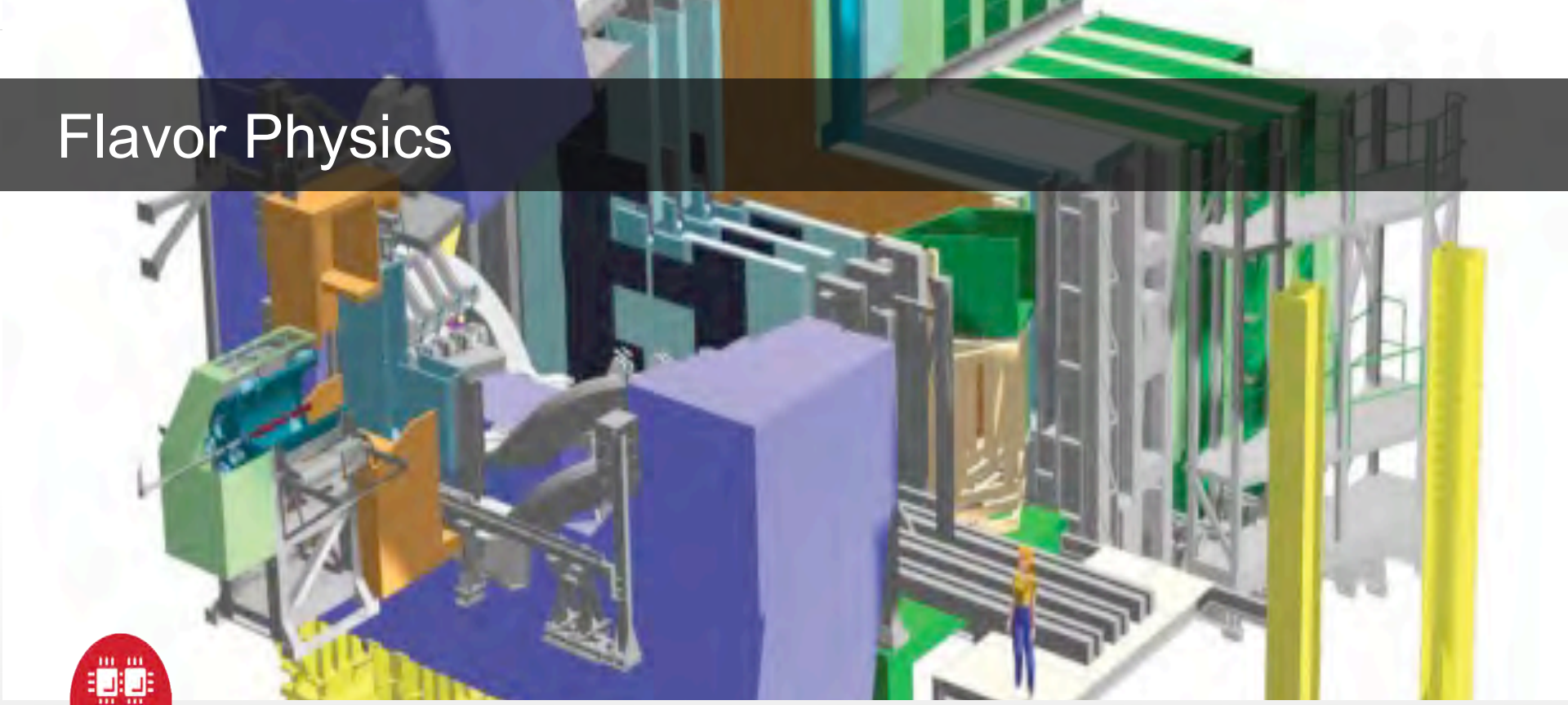
Mapping

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

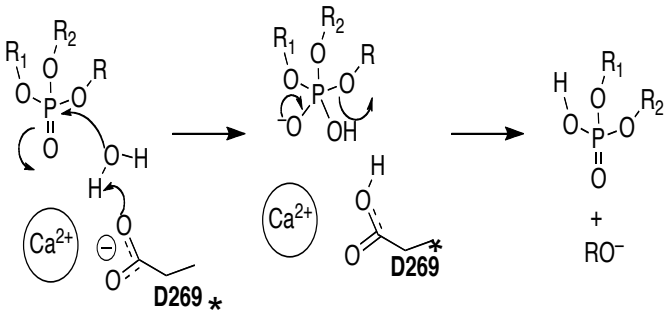
Flavor Physics

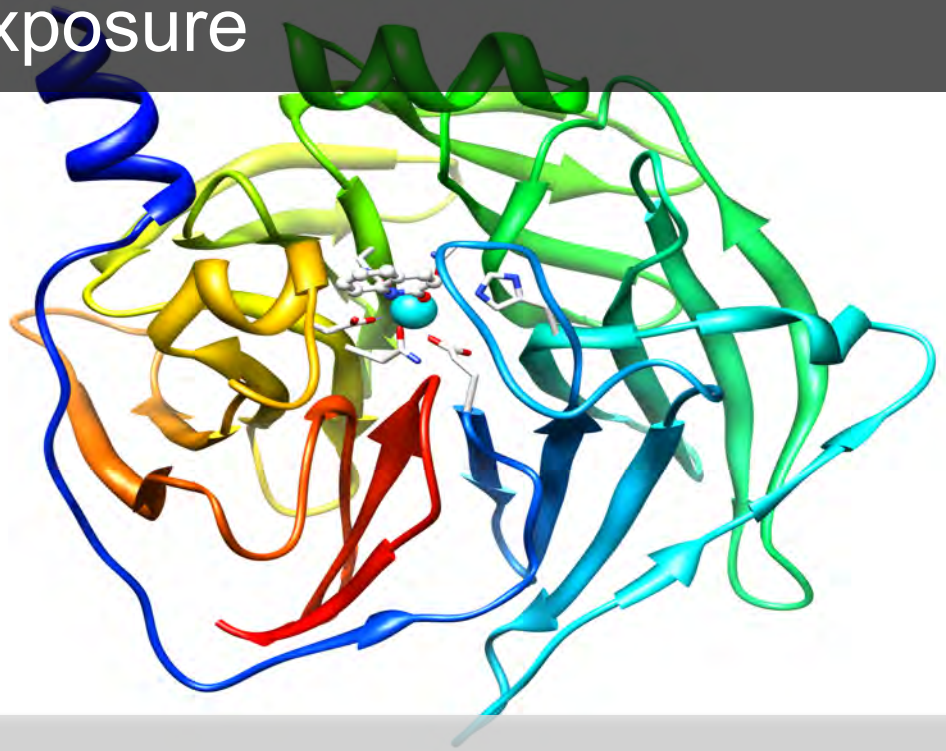


A researcher accesses OSC services to answer basic questions about the universe by modeling very high-mass particles, called quarks, which have six variations known as flavors

PI: Michael Sokoloff, Univ. of Cincinnati

Treating Nerve Agent Exposure

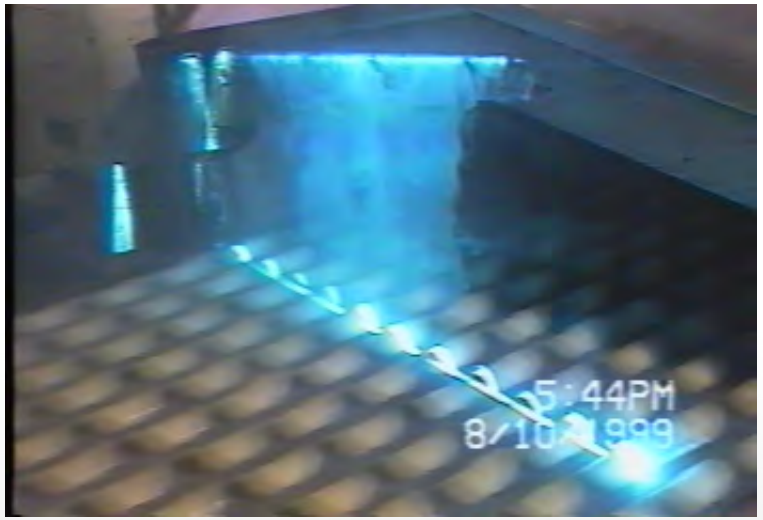


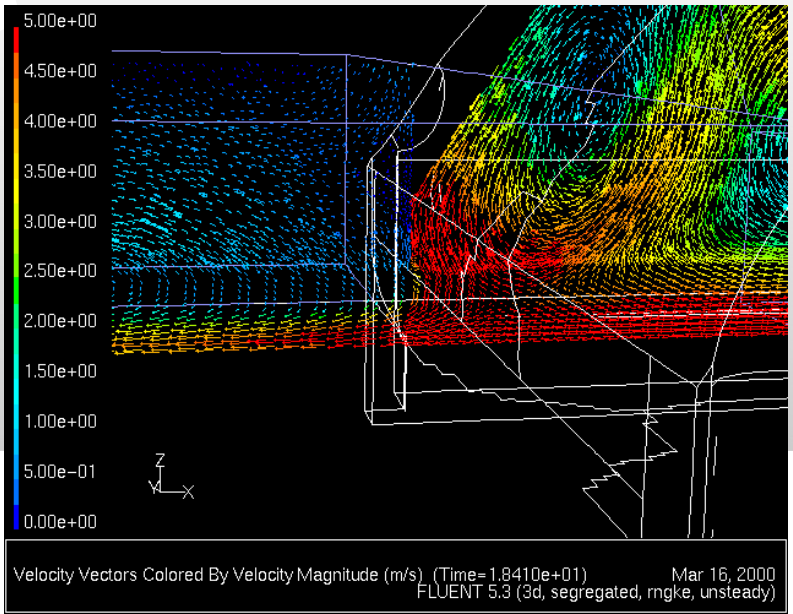


With the power of OSC computing services, a team studies how to capture and destroy organophosphorus nerve agents using modified proteins.

PI: Christopher Hadad, Ohio State University

How to make a billion pringles?





What is the difference between your laptop and a supercomputer?

X 10000 =

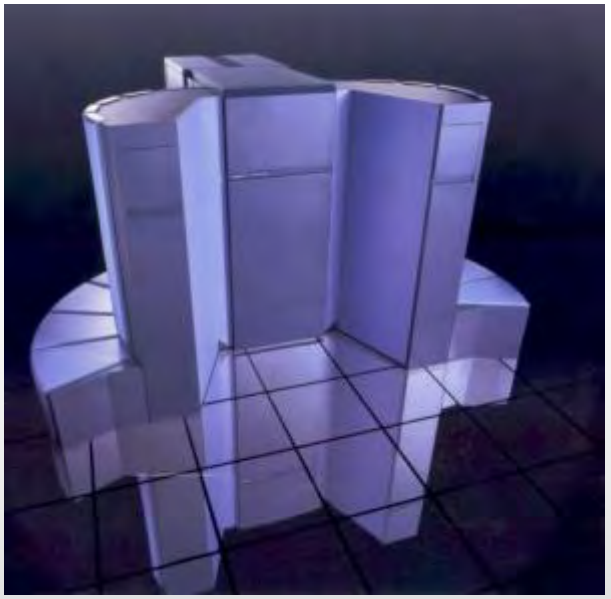
Remote Connect

Supercomputers become history quickly!

Smartphone - 2015

$740	Cost	**$20,000,000**
4 GB	Memory	**128** MB
64 GB	Storage	**30** GB
302 GFLOPS	Speed	**2** GFLOPS

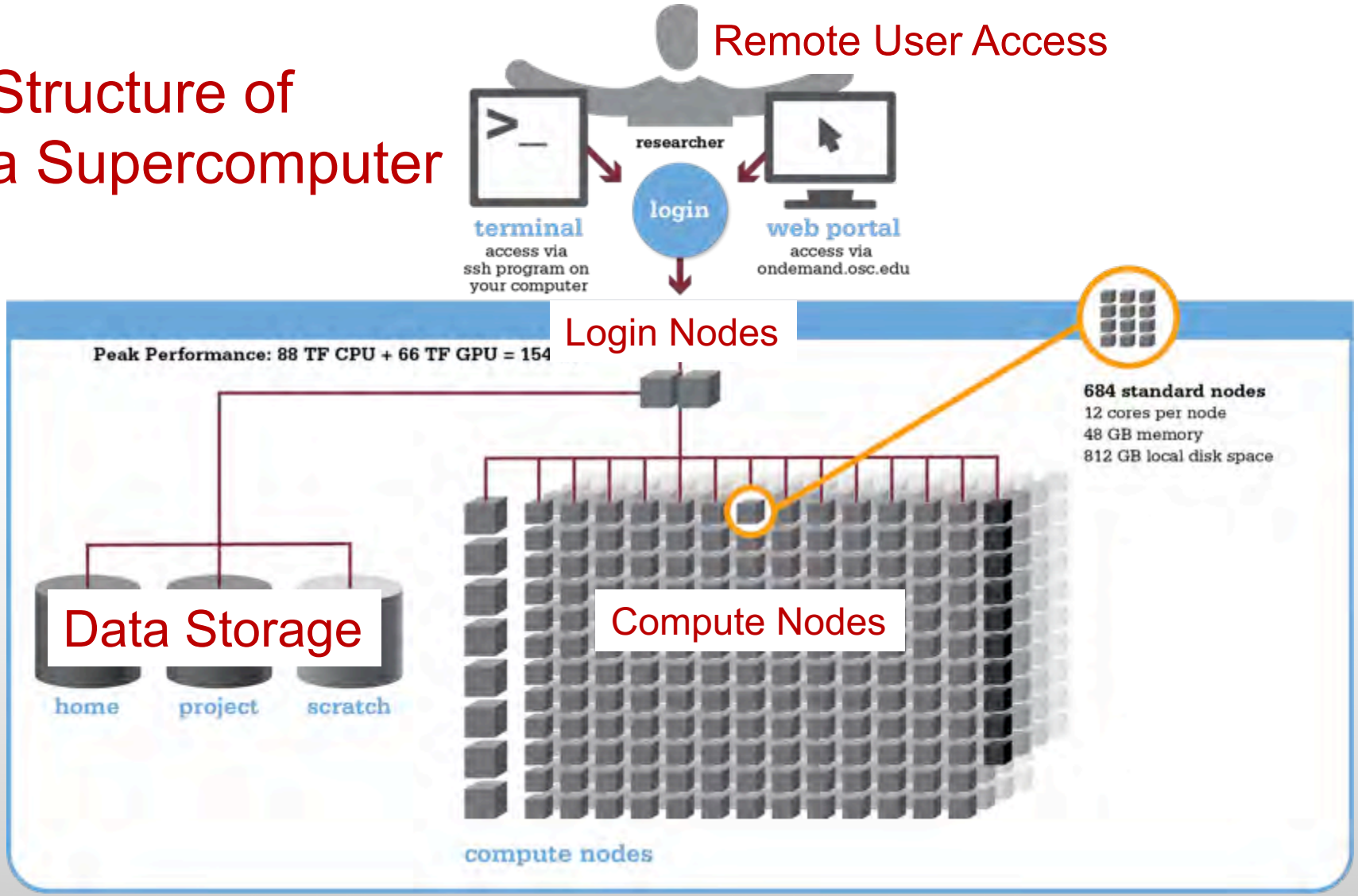
Supercomputer - 1989



HPC Terminology

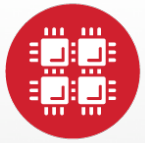
- Cluster
  - A group of computers (nodes) connected by a high-speed network, forming a supercomputer
- Node
  - Equivalent to a high-end workstation, part of a cluster
- Core
  - A processor (CPU), multiple cores per processor chip
- FLOPS
  - “FLoating-point Operations (calculations) Per Second”

Structure of a Supercomputer



Big Numbers

Prefix byte = 1 grain of rice	Relation to HPC
• K (cup of rice) – kilo, 10^3, thousand • M (8 bags of rice) – mega, 10^6, million • G (3 trucks full) – giga, 10^9, billion • T (2 container ships) – tera, 10^{12}, trillion • P (covers Manhattan island) – peta, 10^{15}, quadrillion • E (covers the UK 3x) – exa, 10^{18}, quintillion	• 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



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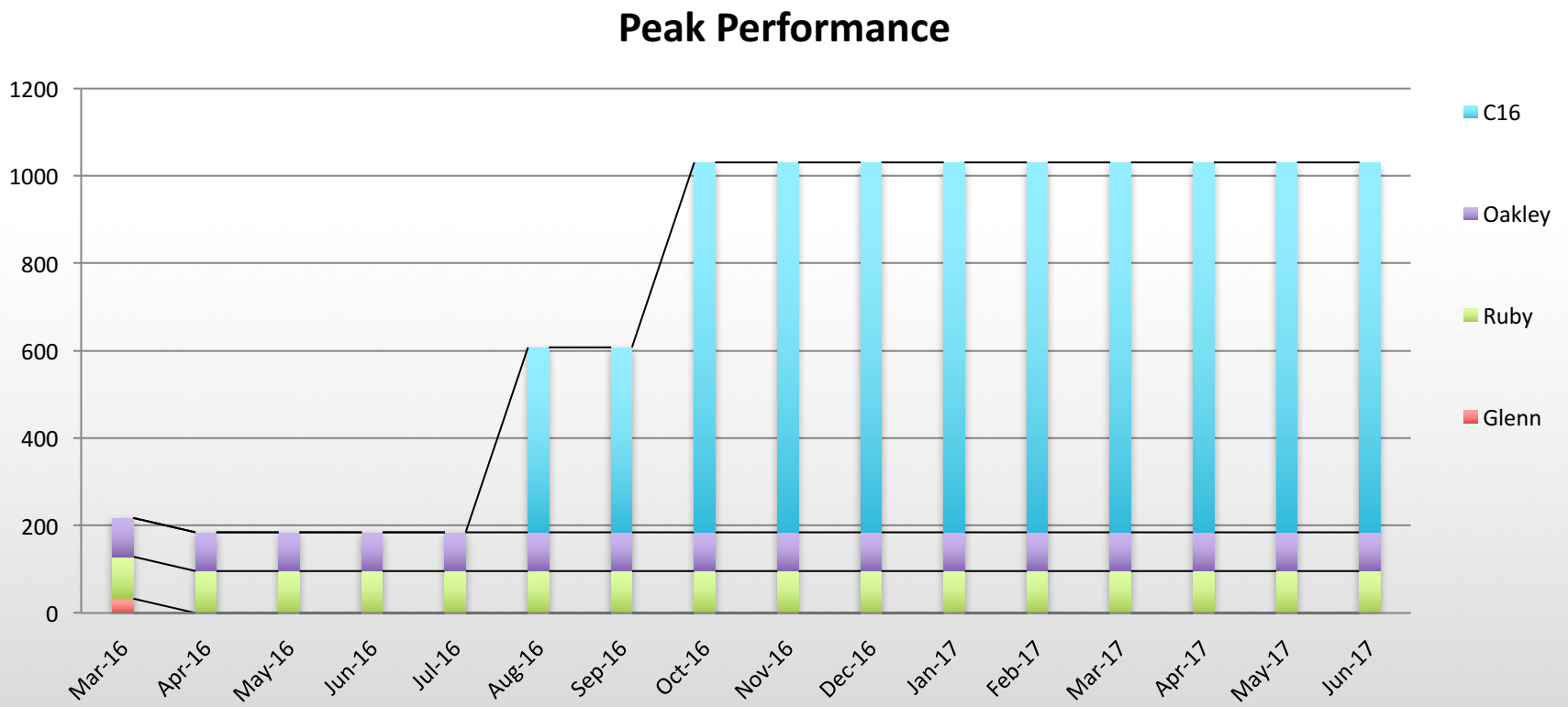
Hardware Overview

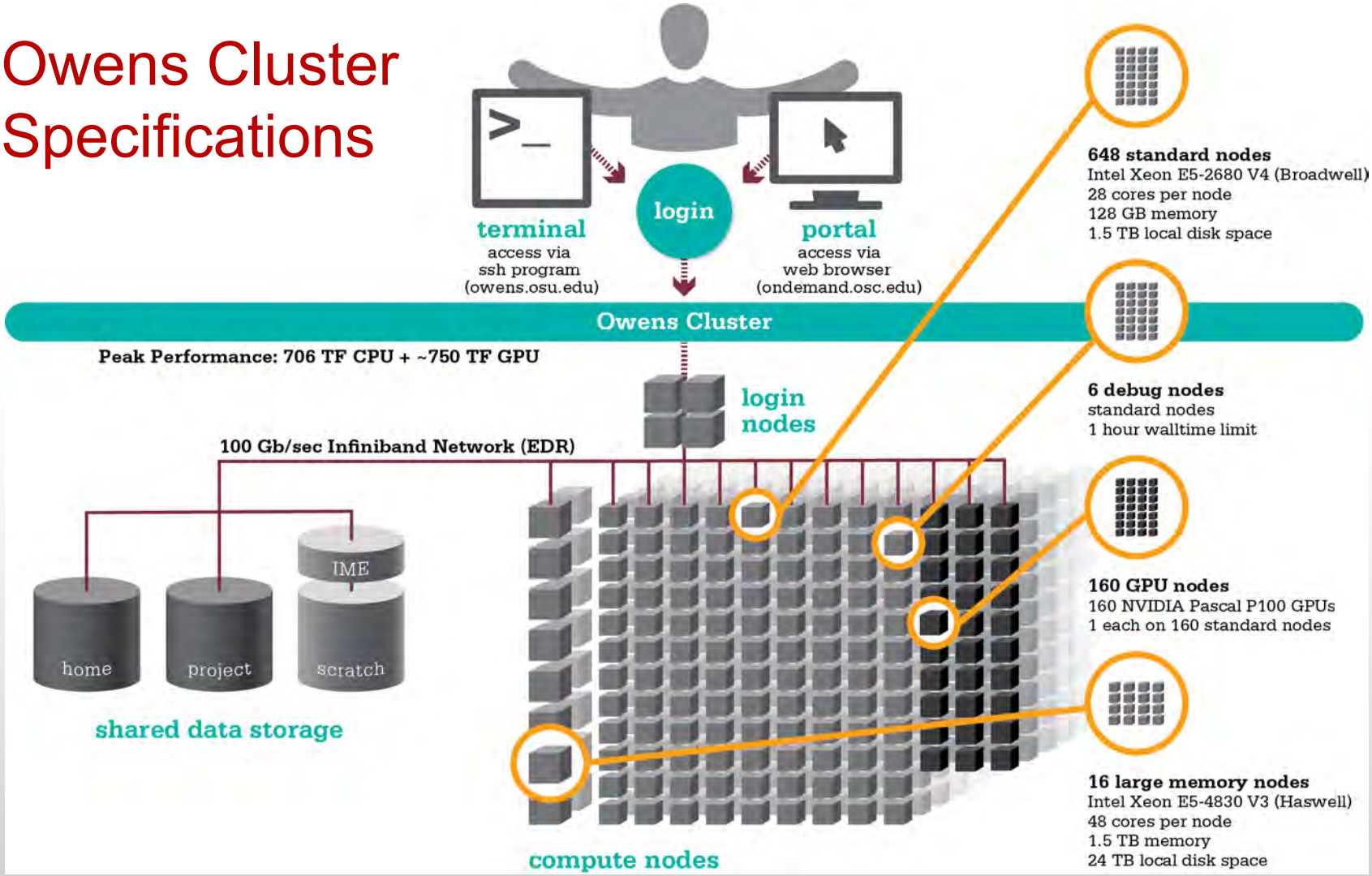
System Configurations

	Owens (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

Owens – Our Newest Cluster 5x Performance Increase

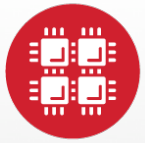


Owens Cluster Specifications



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!



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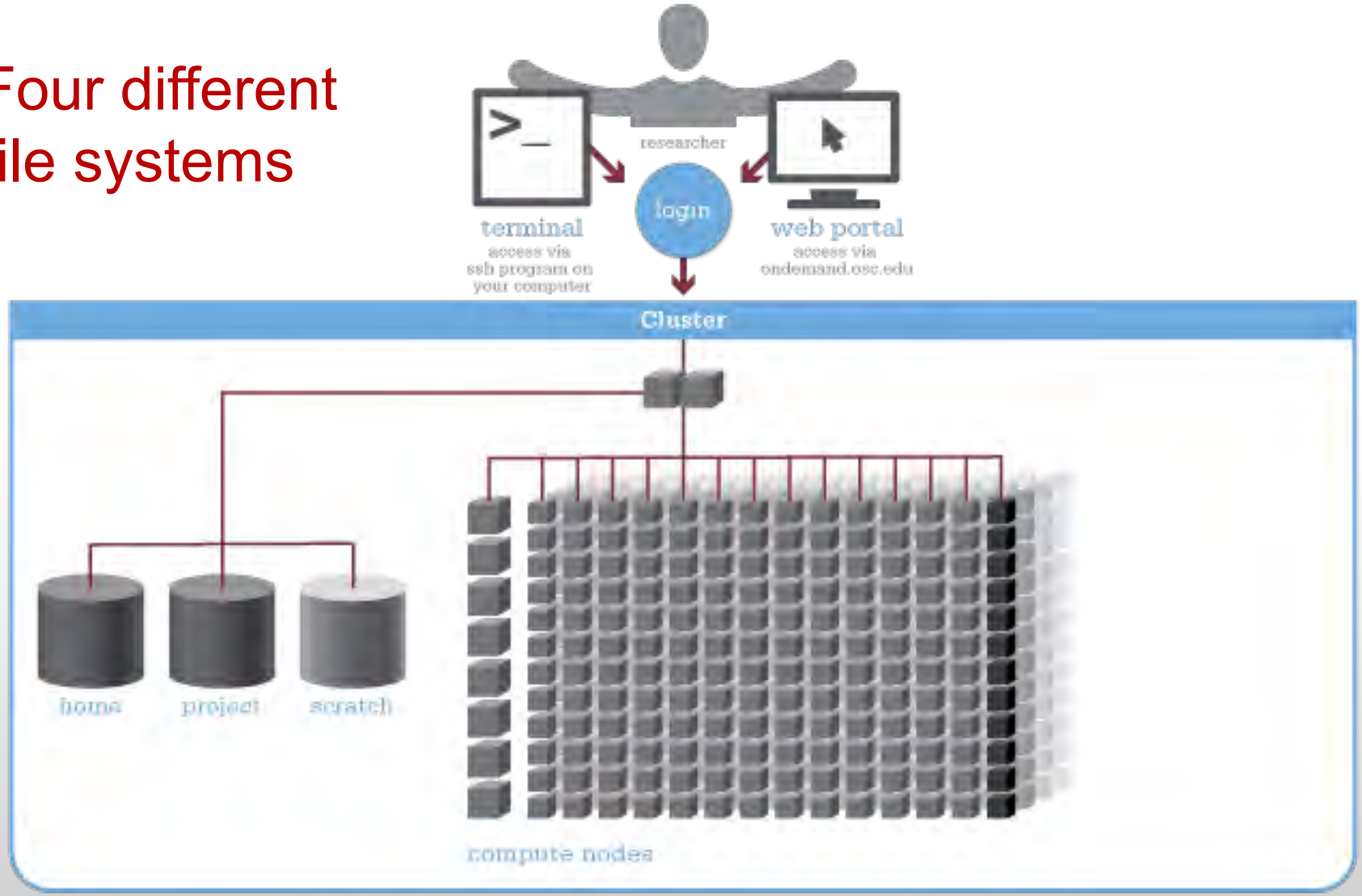
Data Storage Systems

Four different file systems



Filesystem Overview

- Home
  - Store your files here, backed up daily
  - Use $HOME or ~*username* to reference location
- Project
  - Available to Project PIs by request; shared by all users on a project, backed up daily
  - Use /fs/project/*project#* to reference location
- Scratch
  - Store large input or output files here
  - Faster I/O than Home or Project
  - Temporary storage, not backed up
- $TMPDIR
  - Storage on compute nodes, for use during your batch job
  - Be sure to copy any results back to Home at the end of your job, all data purged when job quits

Filesystem	Quota	Backed-Up?	Purged?
Home ($HOME)	500GB	Yes	No
Project (/fs/project)	By request	Yes	No
Scratch (/fs/scratch)	None	No	Yes – 120 days
Compute ($TMPDIR)	800GB (Oakley), 1 TB (Ruby & Owens)	No	Yes – when job completes

File Management

- If you are concerned about Home directory quotas:
  - Compress large, rarely used files
    - Use **`gzip`** or **`bzip2`** commands
  - Combine large numbers of small files into an archive
    - Use **`tar`** command
  - Request Project space for your group (PIs only)
    - Large requests are reviewed by allocations committee
    - Contact OSC Help to initiate request

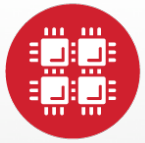
Sample Quota Display

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
```



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User Environment

User Environment Topics

- Connecting to the clusters
- Transferring Files

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

Connecting to the clusters

- 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)

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

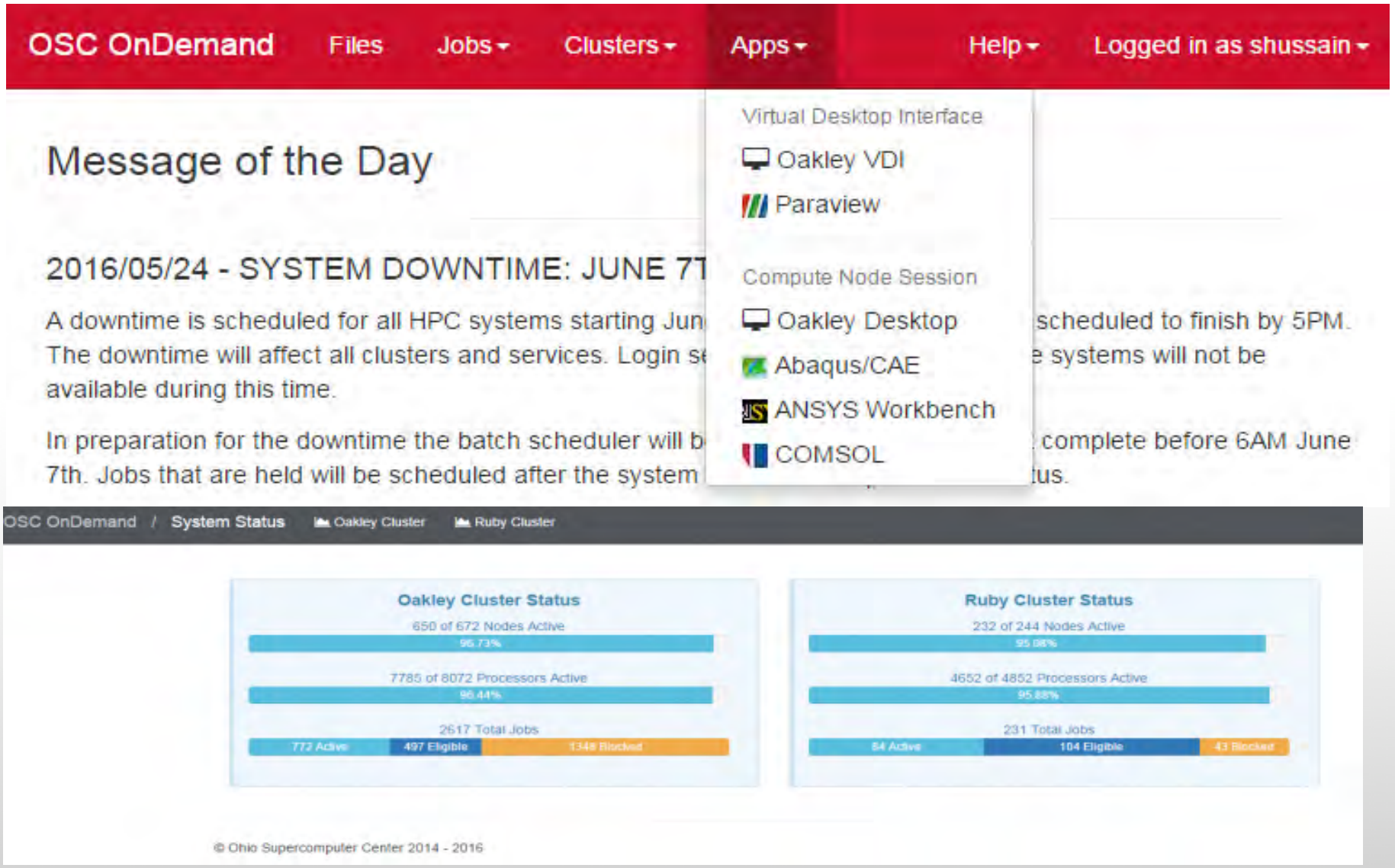
  `ssh -X userid@oakley.osc.edu`
- Windows: Need extra software
  - Both commercial and free versions are available
  - Configure your ssh client to tunnel or forward X11
- Primarily used with programs on login node
  - Can also use with interactive batch jobs

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 (Abaqus, Ansys, Comsol, Paraview)
  - Terminal Access

Tutorial available at

osc.edu/ondemand


OSC OnDemand
Files
Jobs
Clusters
Apps
Help
Logged in as shussain
Virtual Desktop Interface
Oakley VDI
Paraview
Compute Node Session
Oakley Desktop
Abaqus/CAE
ANSYS Workbench
COMSOL
Message of the Day
2016/05/24 - SYSTEM DOWNTIME: JUNE 7T
A downtime is scheduled for all HPC systems starting Jun
scheduled to finish by 5PM.
The downtime will affect all clusters and services. Login s
e systems will not be
available during this time.
In preparation for the downtime the batch scheduler will b
complete before 6AM June
7th. Jobs that are held will be scheduled after the system
tus.
OSC OnDemand / System Status
Oakley Cluster
Ruby Cluster
Oakley Cluster Status
650 of 672 Nodes Active
96.73%
7785 of 8072 Processors Active
96.44%
2617 Total Jobs
772 Active
497 Eligible
1348 Blocked
Ruby Cluster Status
232 of 244 Nodes Active
95.08%
4652 of 4852 Processors Active
95.88%
231 Total Jobs
84 Active
104 Eligible
43 Blocked
© Ohio Supercomputer Center 2014 - 2016

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 - FileZilla
- 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)

File Permissions

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

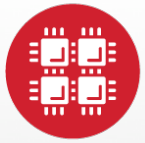
```
-rw-r--r--   1 osu7824 PAS0925   10839 Jan 13  2015 triarm_VVVacid.sdf
-rw-r--r--   1 osu7824 PAS0925   11667 Jan 13  2015 triarm_VVVester.sdf
drwxr-xr-x   8 osu7824 PAS0925    4096 Jan 16  2014 tutorial
-rw-r-x---   1 osu7824 PAS0925 9917889 Jan 15  2015 ValBaskEst32_gopt.log
-rw-r--r--   1 osu7824 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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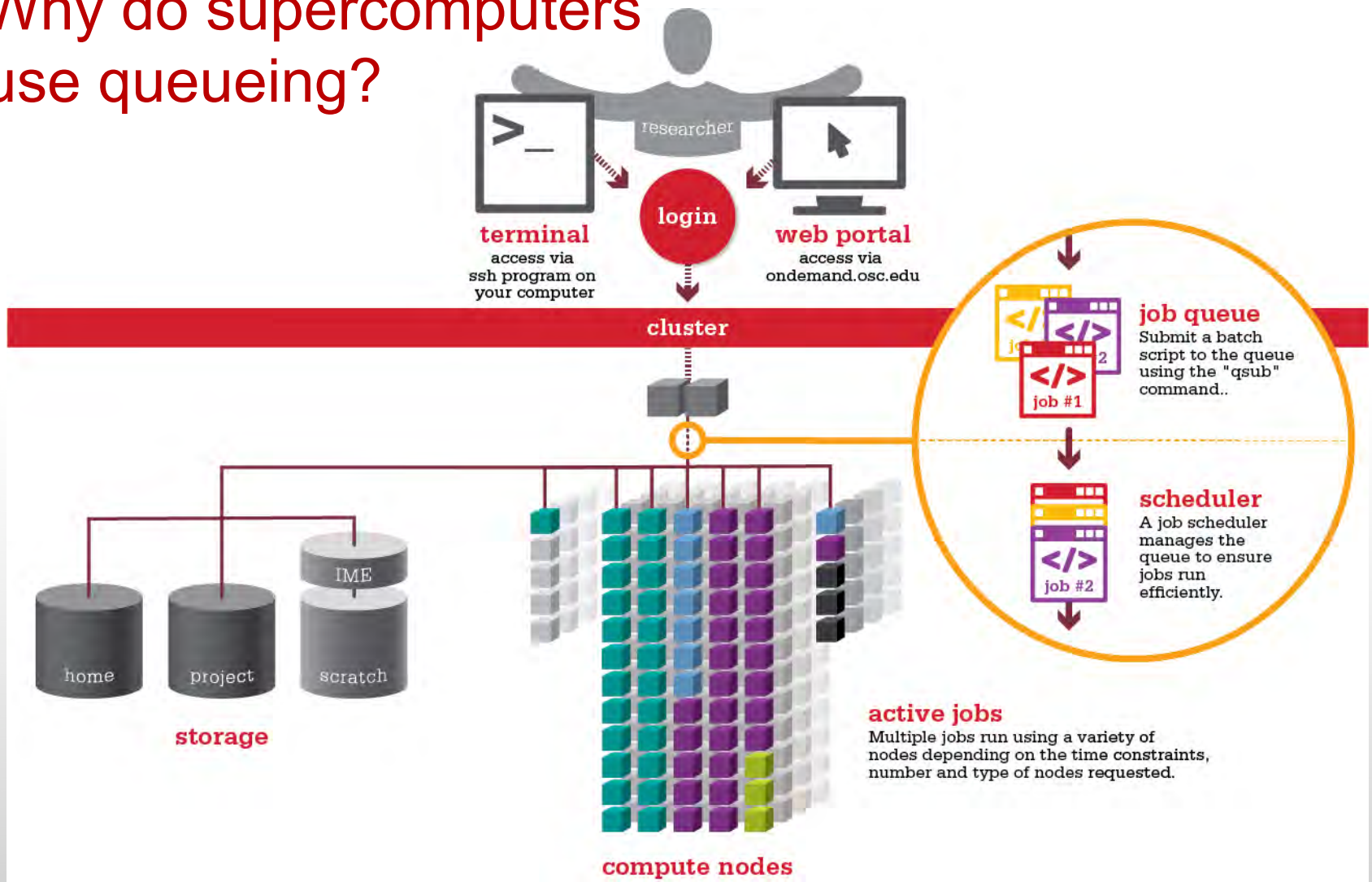
Batch Processing

Why do supercomputers use queueing?



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

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

Steps for Running a Job on the Compute Nodes

1. Create a batch script for a job
2. Submit the job
3. Job gets queued
4. Job runs when resources become available
5. 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=28
#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***

List of Batch commands on osc.edu

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

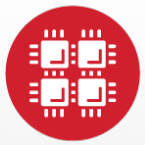
- Interactive, but handled through batch system
  - Resource limits same as standard batch limits
- Useful for tasks forbidden on login nodes
  - Debug parallel programs
  - Run a GUI program that's too large for login node
- May not be practical when system load is high
  - Long wait, same as standard batch job
- To submit an interactive batch job (example)
  - `qsub -I -X -l nodes=2:ppn=28 -l walltime=1:00:00 -m abe`

Batch Queues

- The three clusters 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 (≤ 1 hour)
  - Special flag required on Ruby and Owens: -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



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Loading and Running Software

Modules for Software access

- 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`**

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

Third party applications

- **General programming software (**$statewide licensed)
  - gnu compilers and debugger
  - $ Intel compilers
  - $ Totalview debugger
  - $ Allinea profiler
  - 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

Access to Licensed Software

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

- List of 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

Resources to get your questions answered

- FAQs & HOWTOs on osc.edu
  - https://www.osc.edu/resources/getting_started/supercomputing_faq
  - https://www.osc.edu/resources/getting_started/howto

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

Demo

- Website tour: www.osc.edu
- MyOSC: https://my.osc.edu/
- OnDemand: ondemand.osc.edu
  - https://www.osc.edu/ondemand

Questions

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