Ohio Supercomputer Center

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Introduction to Projects at OSC

Kate Cahill
Education & Training Specialist

Last Week's Presentation

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

https://www.osc.edu/~kcahill/NewUser

Overview

- Jobs suited to OSC resources
- Condos at OSC
- How to get an allocation
- Other HPC resources to consider

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Types of Jobs suited to OSC resources

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

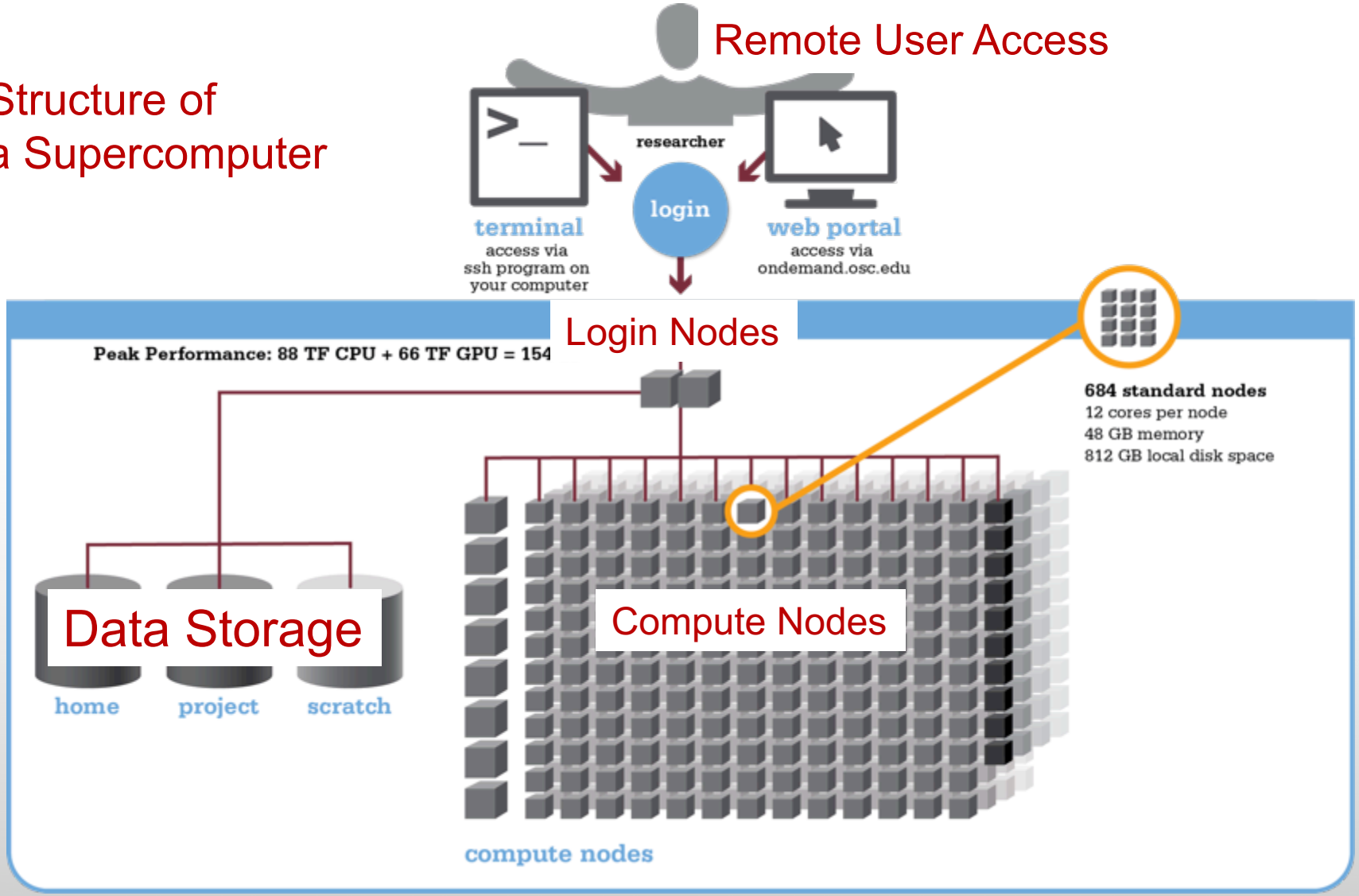
Memory

- Holds data that is being calculated on, as well as computational instructions
- *Shared memory* is local to one node and several process threads can share the same data addresses.
- *Distributed memory* is on multiple nodes and each process normally has its own copy or part of the data.

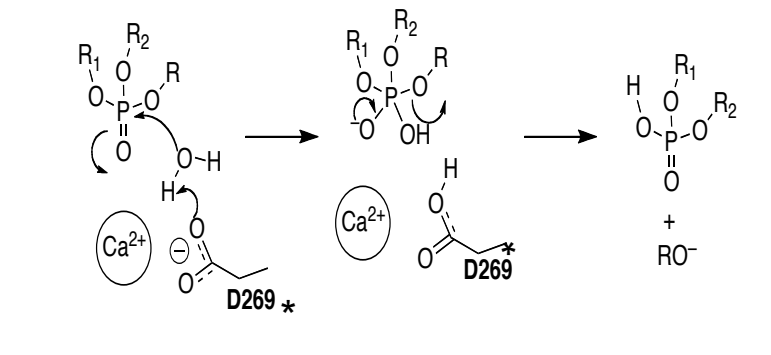
Storage

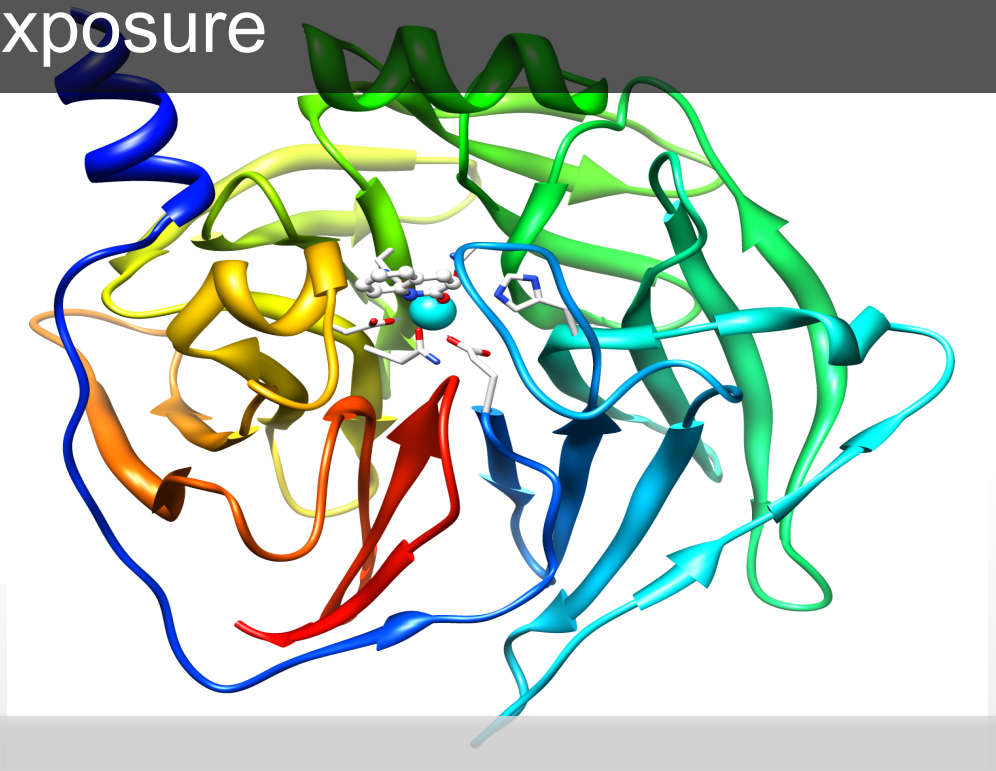
- Home
  - Store your files here, backed up daily
  - Use $HOME or ~*username* to reference location
- Project
  - Available to Project PIs by request; shared by all users on a project, backed up daily
  - Use /fs/project/*project#* to reference location
- Scratch
  - Store large input or output files 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

Structure of a Supercomputer



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

OSC Supercomputers + Storage

	Owens (2016)	Ruby (2014)	Oakley (2012)
Theoretical Performance (TF)	~1600	~144	~154
# Nodes	824	240	692
# CPU Cores	23,392	4,800	8,304
Total Memory (TB)	~120	~15.3	~33.4
Memory per Core (GB)	4.5	3.2	4
Interconnect Fabric (IB)	EDR	FDR/EN	QDR

	Home (2016)	Project (2016)	Scratch (2016)	Tape (2010-17)
Capacity (PB)	0.8	3.4	1.1	5+
Bandwidth (GB/s)	10	40	100	3.5

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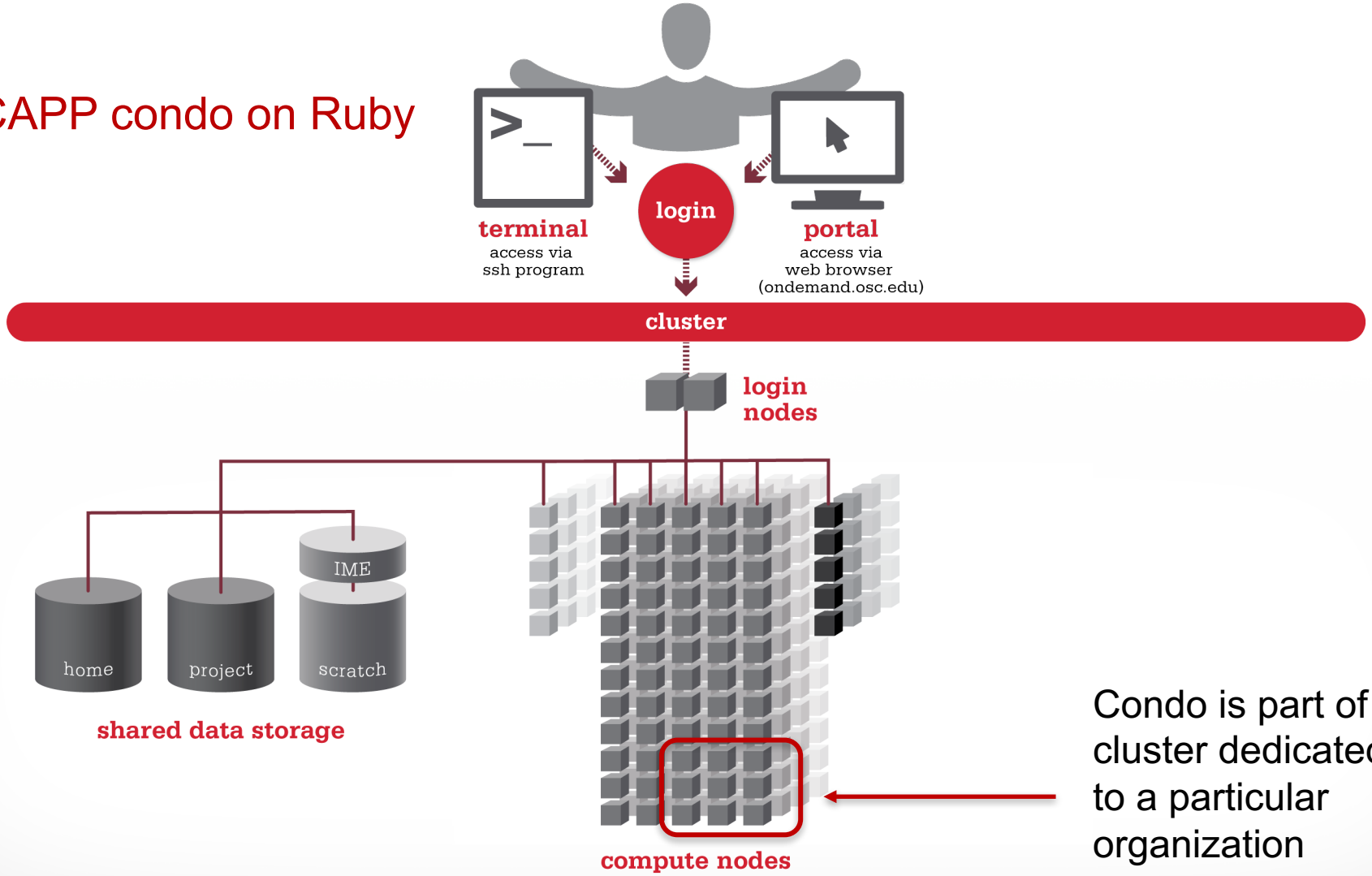
Condos at OSC – CCAPP condo

CCAPP condo on Ruby



Condo is part of cluster dedicated to a particular organization

Condo Benefits

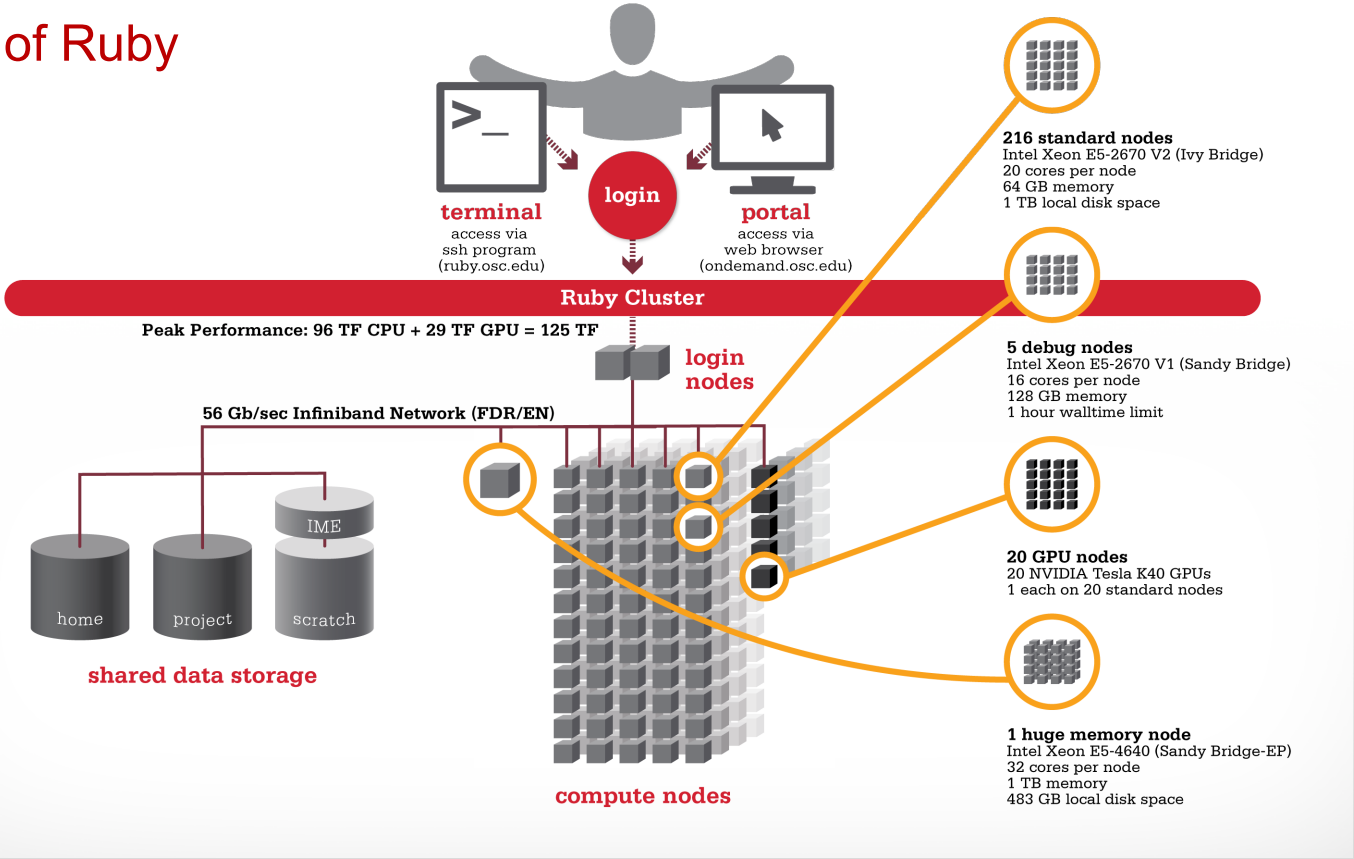
To Users

- Administration handled by OSC experts
- Can leverage OSC infrastructure
- Cost savings due to vendor relationships and volume purchasing
- Priority access to condo resources
- 24/7 support

To OSC

- Expand resources
- Revenue allows investment in staff
- “Backfill” on idle condo nodes can be used to provide cycles that would otherwise be “wasted” to the broader community

Features of Ruby Cluster



CCAPP condo structure

- Detailed system specifications:
- 21 total nodes on Ruby
  - 20 cores per node
  - 64 GB of memory per node
  - 1 TB of local disk space
- Intel Xeon E5 2670 V2 CPUs
- HP SL250 Nodes
- FDR IB Interconnect
  - Low latency
  - High throughput
  - High quality-of-service

How to use CCAPP condo efficiently

- Ruby uses full node scheduling
- Most condZZZ accounts can only access condo resources

- Jobs that only use 1 processor at a time should be bundled so the whole node is in use

- **Projects that require 1000s jobs or 1000s nodes are not suited for this condo**

See: https://www.osc.edu/~kmanalo/multithreadedsubmission
(and next week's presentation)

Batch Script Commands

```
Job Name:              #PBS -N serial_fluent
Wall time:             #PBS -l walltime=1:00:00
Nodes and cores:       #PBS -l nodes=1:ppn=28
Project:               #PBS -A PCON0003
Outfile format:        #PBS -j oe
Software request:      #PBS -l software=fluent+1
Email notifications:#PBS -m abe
```

If you are on more than one project, your job will not submit without explicit project included

Check projects using `groups` ***`username`***

Get more batch commands here: http://go.osu.edu/B6WJ

Updated information on condo

- For more information and updates, CCAPP condo information page at osc.edu:

- https://www.osc.edu/supercomputing/computing/ruby/ccapp_condo

- Presentations will be posted here

- Updates on condo resources

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How to get an allocation

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 to Ohio academic users
- Commercial projects
  - 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
  - OWENS 1 resource unit (RU) = 10 CPU hours
  - OAKLEY & RUBY 1 resource unit (RU) = 20 CPU hours
  - CPU hour = walltime x (total # of cores requested)
- Project receives an allocation of RUs
- Jobs are charged to a project

Requesting a New Project- https://www.osc.edu/supercomputing/support/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)
- Classroom account

Start-up application https://app.osc.edu/cgi-bin/app/startup

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Submit an Application

Select the type of application.

Instructions:

Startup projects are available to eligible new researchers. They include login accounts on all of OSC's high-performance computers and 5000 resource units.

Fill out each of the 3 sections in sequence by clicking on the links to the right and following the instructions there. When you have finished with a section, most browsers will display a check mark beside it, indicating that it is done.

If you want to go back and make additions or corrections to data already entered, just click on the link to that section.

Once you have completed all the sections, you will have the option of submitting your application. To do so, just click on the "Submit application" button. Note that this button will not be visible until all other sections are complete.

Glossary of Terms

1 Primary Contact Information
To request a project, you must be a faculty member or research scientist who maintains a full-time position at an Ohio academic institution.

2 Authorized User Information
Here is where you specify additional researchers or students to add to your project.

3 Upload Files
Upload files containing additional information about your project.

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 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

System Status

- Check system status on:
  - Message of the day (/etc/motd) – displayed at login
  - Twitter: @HPCnotices
  - Email for major outages or problems
- Scheduled downtimes
  - Quarterly maintenance – usually 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 next Thursday Sept. 28th at OSC on West Campus

Citing OSC

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

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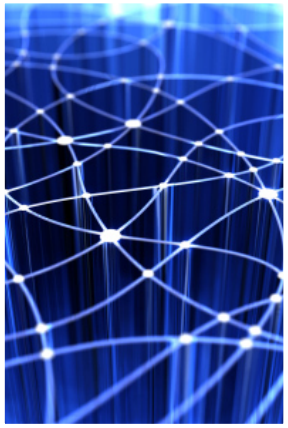
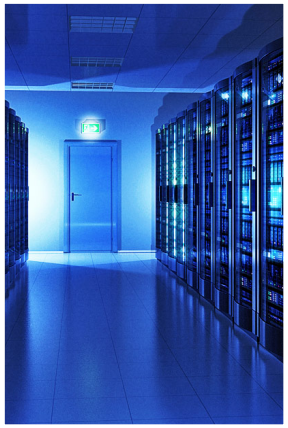
Other HPC resources to consider

What is XSEDE?



Foundation for a National CI Ecosystem

- Comprehensive suite of advanced digital services that federates with other high-end facilities and campus-based resources



Unprecedented Integration of Diverse Advanced Computing Resources

- Innovative, open architecture making possible the continuous addition of new technology capabilities and services

Compute and Analytics Resources

BRIDGES

Featuring interactive on-demand access, tools for gateway building, and virtualization.

SDSC

Comet: hosting a variety of tools including Amber, GAUSSIAN, GROMACS, Lammps, NAMD, and VisIt.

Jetstream

A self-provisioned, scalable science and engineering cloud environment

TACC

Stampede: Intel's new innovative MIC technology on a massive scale

LSU

Super Mic: Equipped with Intel's Xeon Phi technology. Cluster consists of 380 compute nodes.

TACC

Wrangler: Data Analytics System combines database services, flash storage and long-term replicated storage, and an analytics server. IRODS Data Management, HADOOP Service Reservations, and Database instances.

High Throughput Computing

Open Science Grid

- Governed by the OSG consortium
- 126 institutions with ~120 active sites collectively supporting usage of ~2,000,000 core hours per day
- High throughput workflows with simple system and data dependencies are a good fit for OSG
- Access Options:
  - OSGConnect available to any researcher affiliated with US institutions and who are funded by US funding agencies
  - OSG Virtual Organization such as CMS and ATLAS
  - XSEDE
- https://portal.xsede.org/OSG-User-Guide

XSEDE Visualization and Data Resources

Visualization

Maverick@ TACC

- HP/NVIDIA cluster
- 132 TB memory
- VisIt
- ParaView
- Interactive Data Language

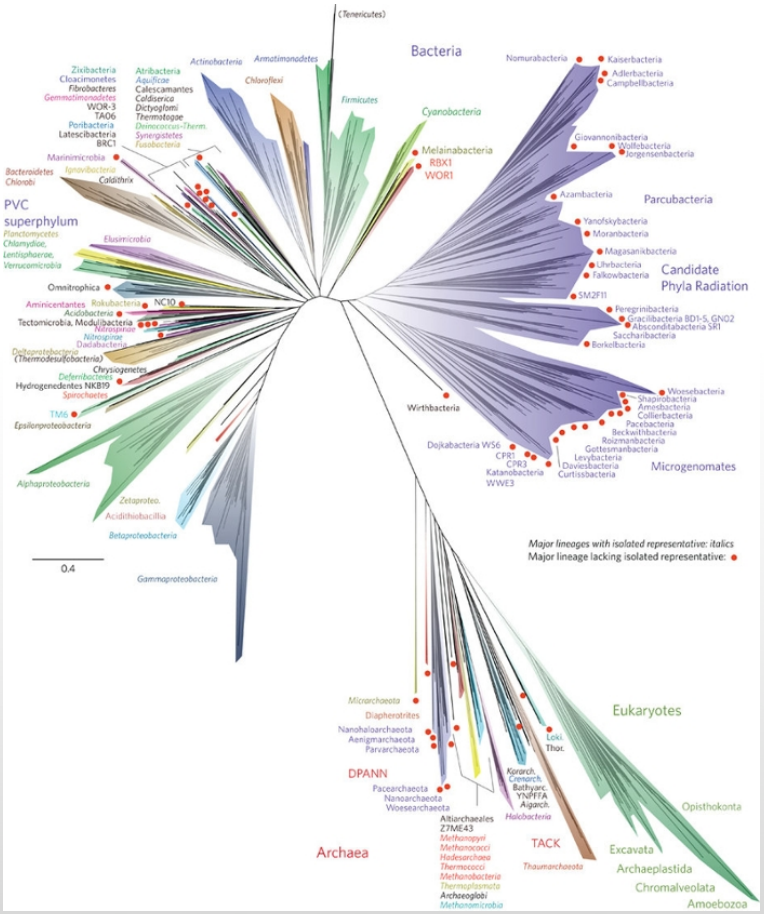
Visualization Portal

- Remote, interactive, web-based visualization
- iPython / Jupyter Notebook integration
- R Studio Integration

Storage

- **Resource file system storage**: All compute/visualization allocations include access to limited disk and scratch space on the compute/visualization resource file systems to accomplish project goals
- **Archival Storage**: Archival storage on XSEDE systems is used for large-scale persistent storage requested in conjunction with compute and visualization resources.
- **Stand-alone Storage**: Stand-alone storage allows storage allocations independent of a compute allocation.

Science Gateways

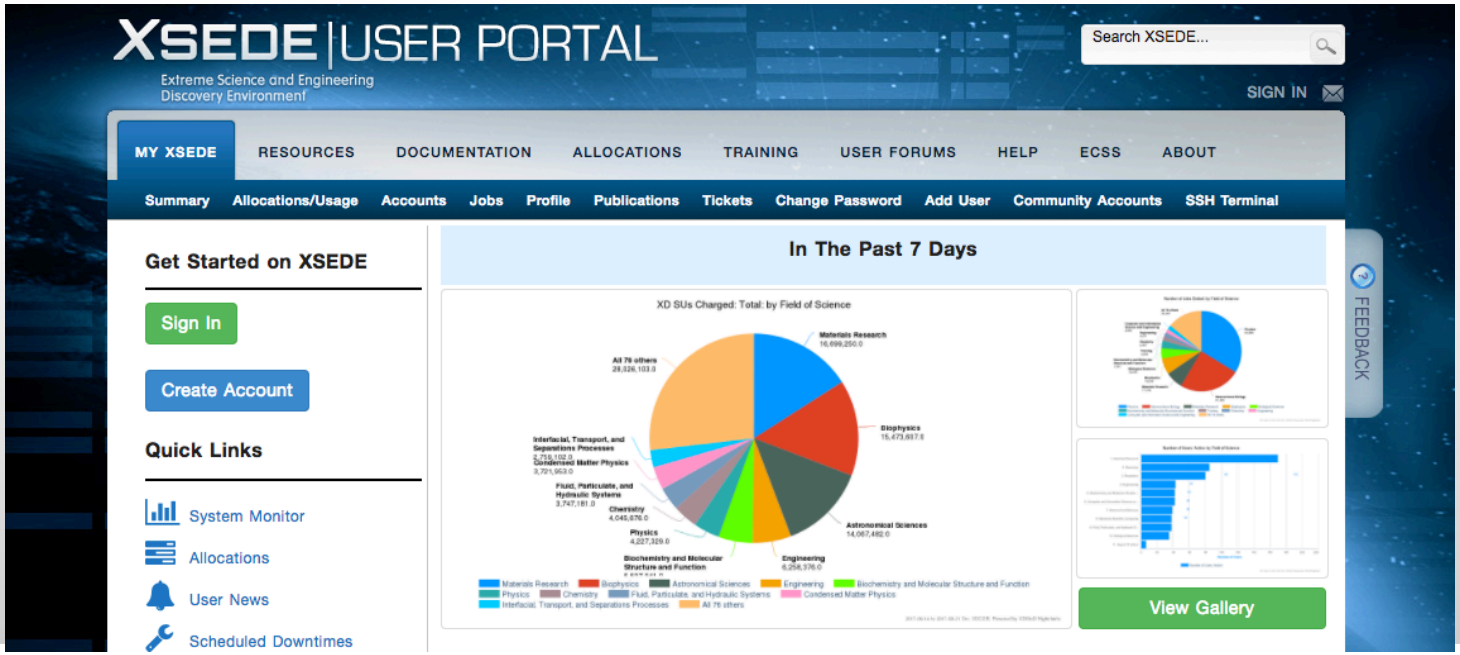


The CIPRES science gateway: A NSF investment launching thousands of scientific publications with no sign of slowing down.

https://sciencenode.org/feature/cipres-one-facet-in-bold-nsf-vision.php?clicked=title

More Information

- XSEDE Website: www.xsede.org
- XSEDE Portal: portal.xsede.org
  - Free live training available on parallel programming: MPI, OpenMP, etc.
  - Free ondemand training on HPC topics & how to get an XSEDE allocation



Important Points to Remember

- The CCAPP condo on Ruby is 21 nodes (420 total processors)
- Ruby uses whole node scheduling (20 processors per node)
- Users on the condo cannot access other OSC clusters
- If your project requires lots of jobs or many large jobs, consider getting a separate allocation
- It is easy to get a start-up grant and relatively painless to renew
- There are even larger HPC resources available through XSEDE

* Next week: How to bundle Jobs for Batch Submission
See these references:
https://www.osc.edu/~kmanalo/multithreadedsubmission
https://www.osc.edu/supercomputing/batch-processing-at-osc

Questions?

Kate Cahill
Education & Training Specialist
Ohio Supercomputer Center
kcahill@osc.edu

You can sign up for one-on-one consultations
go.osu.edu/rc-osc