

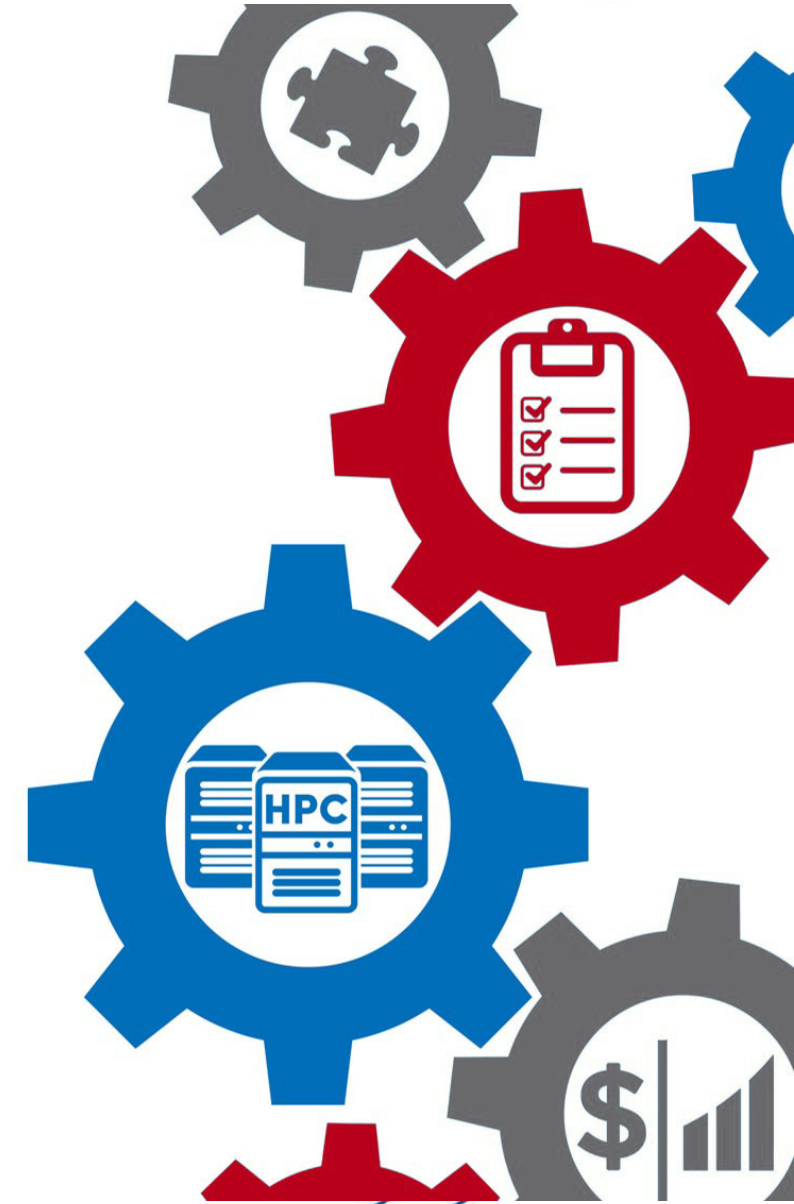


# WELCOME!

IF YOU HAVE NOT ALREADY DONE SO,  
PLEASE FOLLOW SETUP INSTRUCTIONS!

<https://github.com/ubccr/hpc-toolset-tutorial>

- View our “meeting decorum” document  
<https://tinyurl.com/pearc-hpctoolset>
- Join the Slack channel for the tutorial  
<https://tinyurl.com/pearc-slack>



# Open OnDemand, Open XDMoD, and ColdFront: An HPC center management toolset

Tutorial presented at PEARC21 by staff from:  
Ohio Supercomputer Center  
UB Center for Computational Research  
Virginia Tech Advanced Research Computing



**Ohio Supercomputer Center**

An OH·TECH Consortium Member

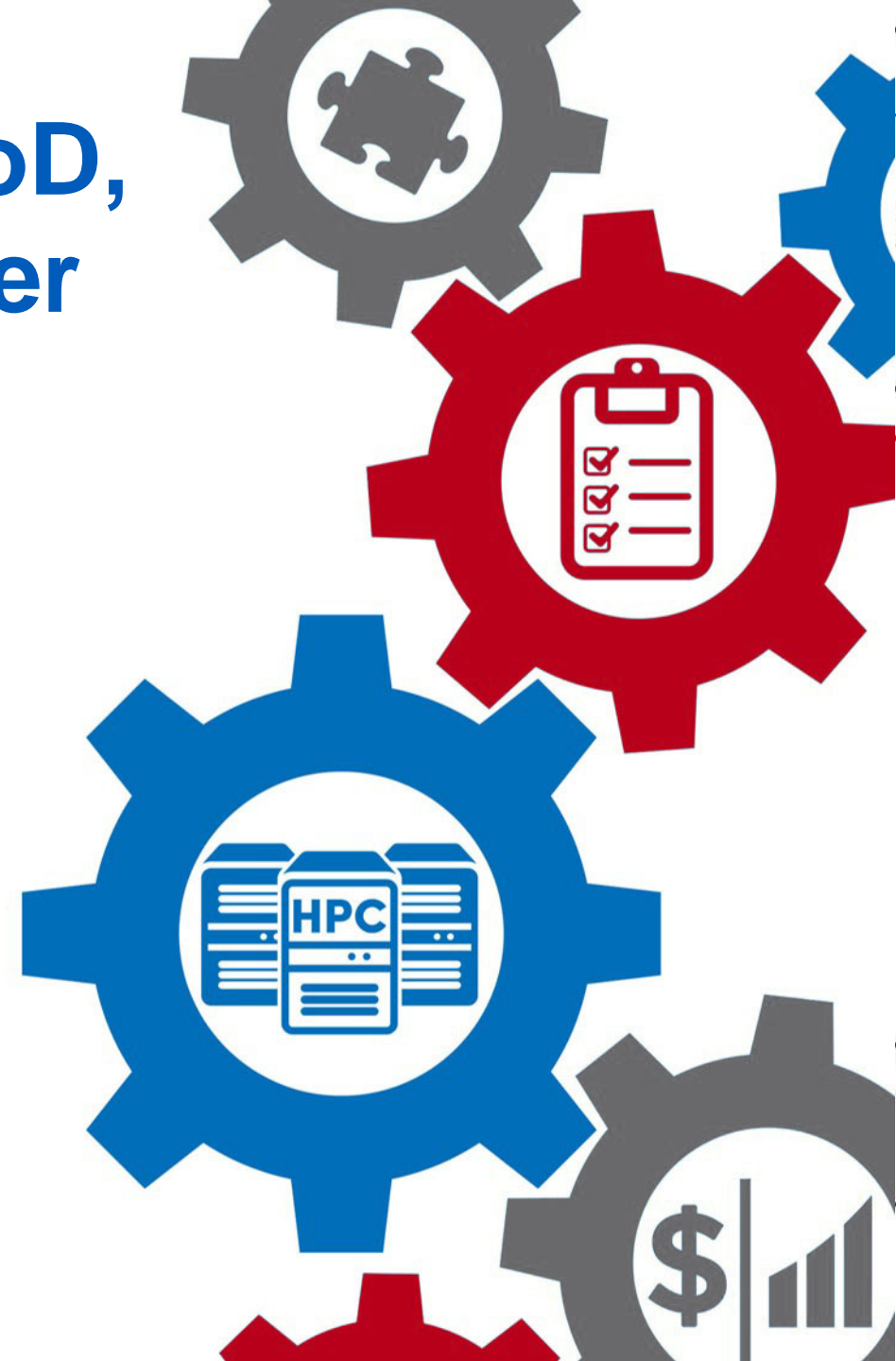


**VIRGINIA  
TECH™**



University at Buffalo

Center for Computational Research





## Tutorial Staff:

Andrew Bruno, UB

Alan Chalker, OSC

Ayush Chaturvedi, VT

Andrew Collins, OSC

Robert DeLeon, UB

Trey Dockendorf, OSC

David Hudak, OSC

Matt Jones, UB

Jeff Ohrstrom, OSC

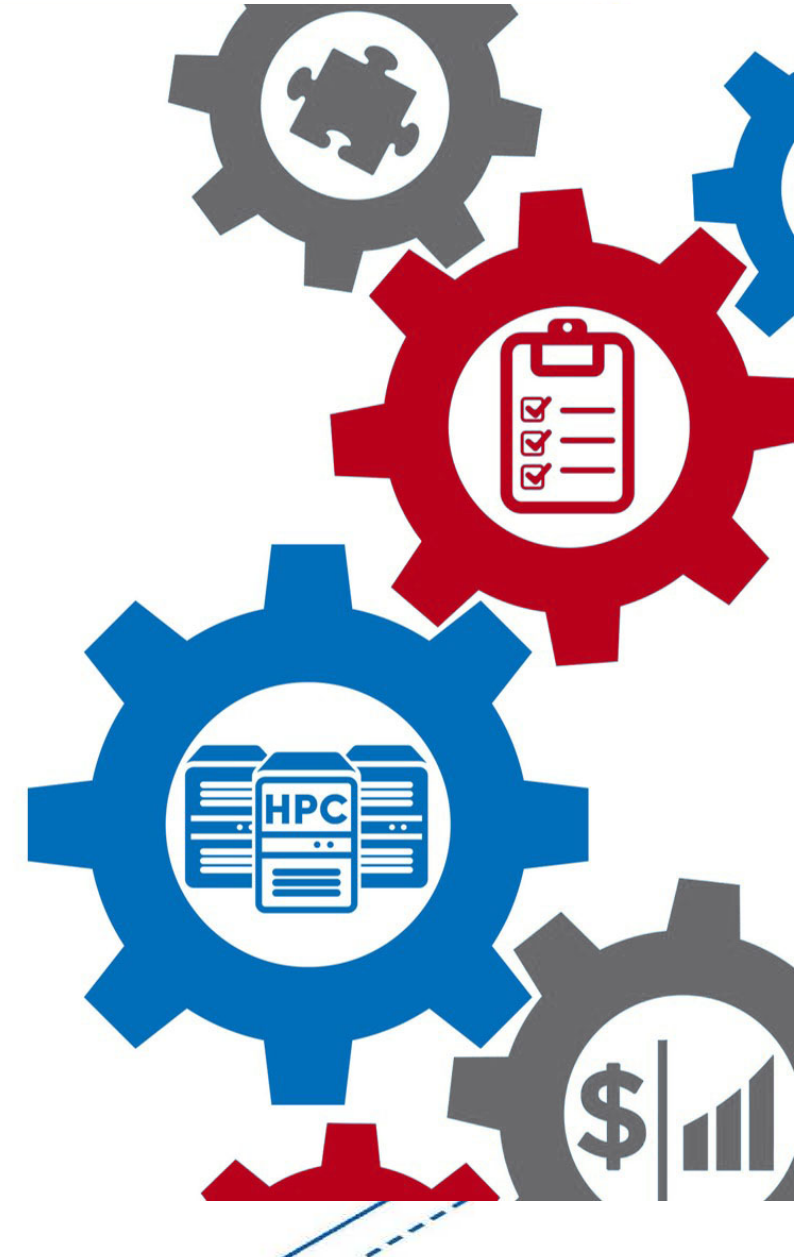
Ryan Rathsam, UB

Travis Ravert, OSC

Dori Sajdak, UB

Bob Settlage, VT

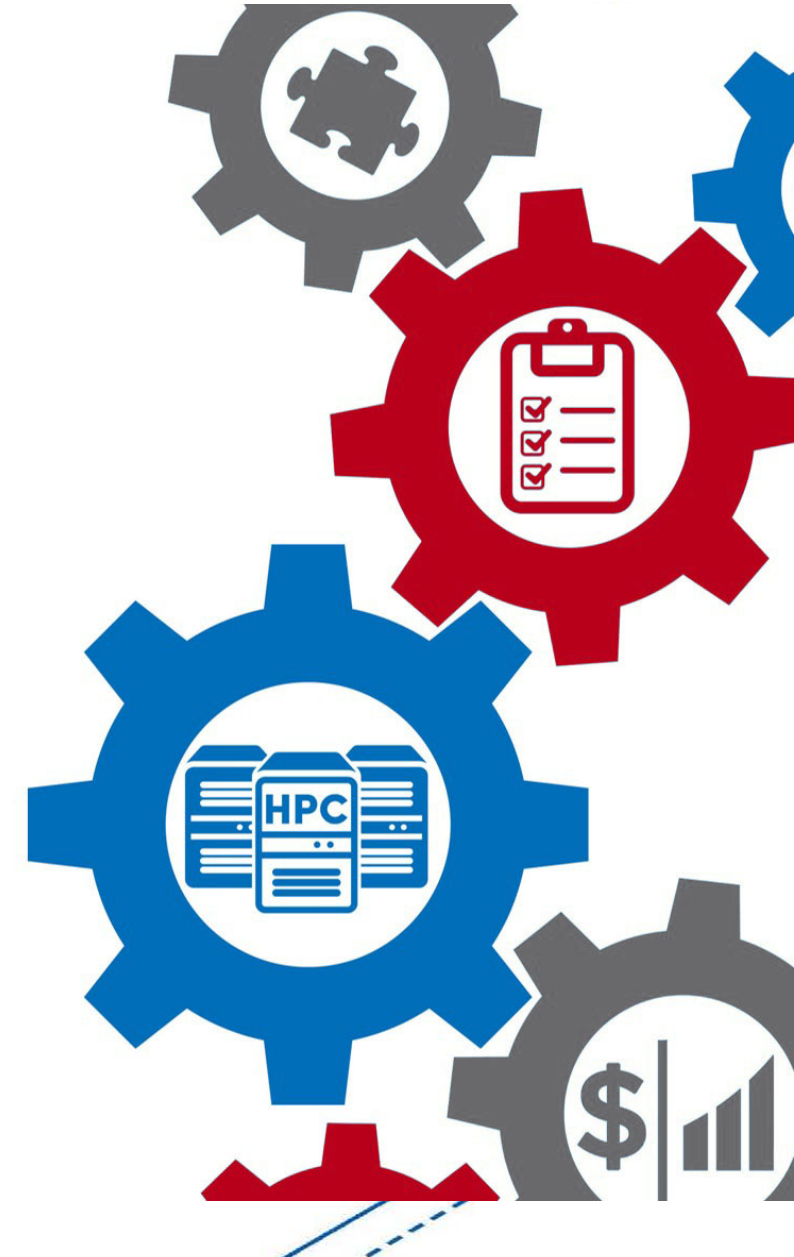
Joseph White, UB





# Agenda

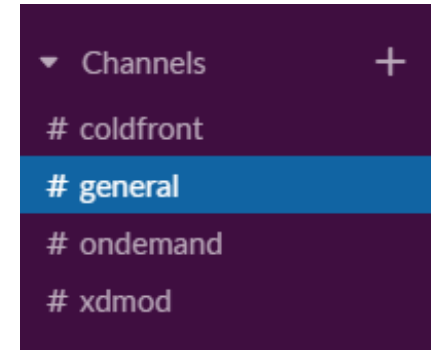
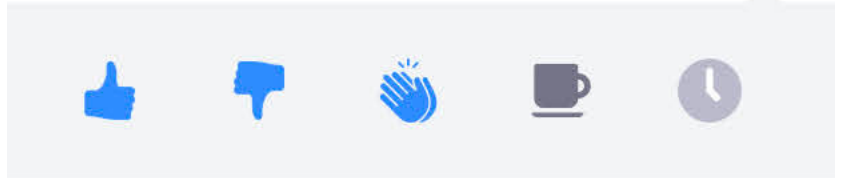
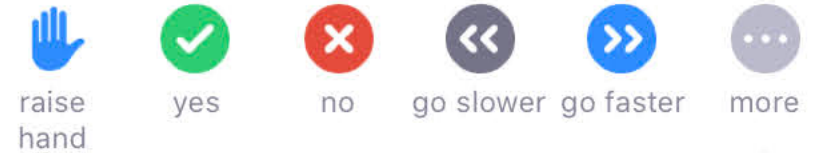
- Getting Started
- Tutorial Goals
- Brief intro on all three products
- Tutorial technology
- Part 1: ColdFront
- Break: 15 minutes
- Part 2: Open XDMoD
- “Lunch” Break – 30 minutes
- Part 3: Open OnDemand
- Part 4: Open OnDemand interactive app configuration
- Break: 15 minutes
- Part 5: Open OnDemand & Open XDMoD integrations
- Post Workshop – breakout sessions & slack channel





## Getting Started

- View our “meeting decorum” document  
<https://tinyurl.com/pearc21-hpctoolset>
  - Please mute yourself & leave your video off
  - Use the “raise hand” button if you have a question & our moderator will unmute you
- Join the Slack channel for the tutorial  
<https://tinyurl.com/pearc-slack>
  - Use Zoom chat only if having trouble with Slack
- Clone the tutorial repo and follow instructions for starting containers  
<https://github.com/ubccr/hpc-toolset-tutorial>
- What to do if you’re having a technical problem – refer to PEARC help

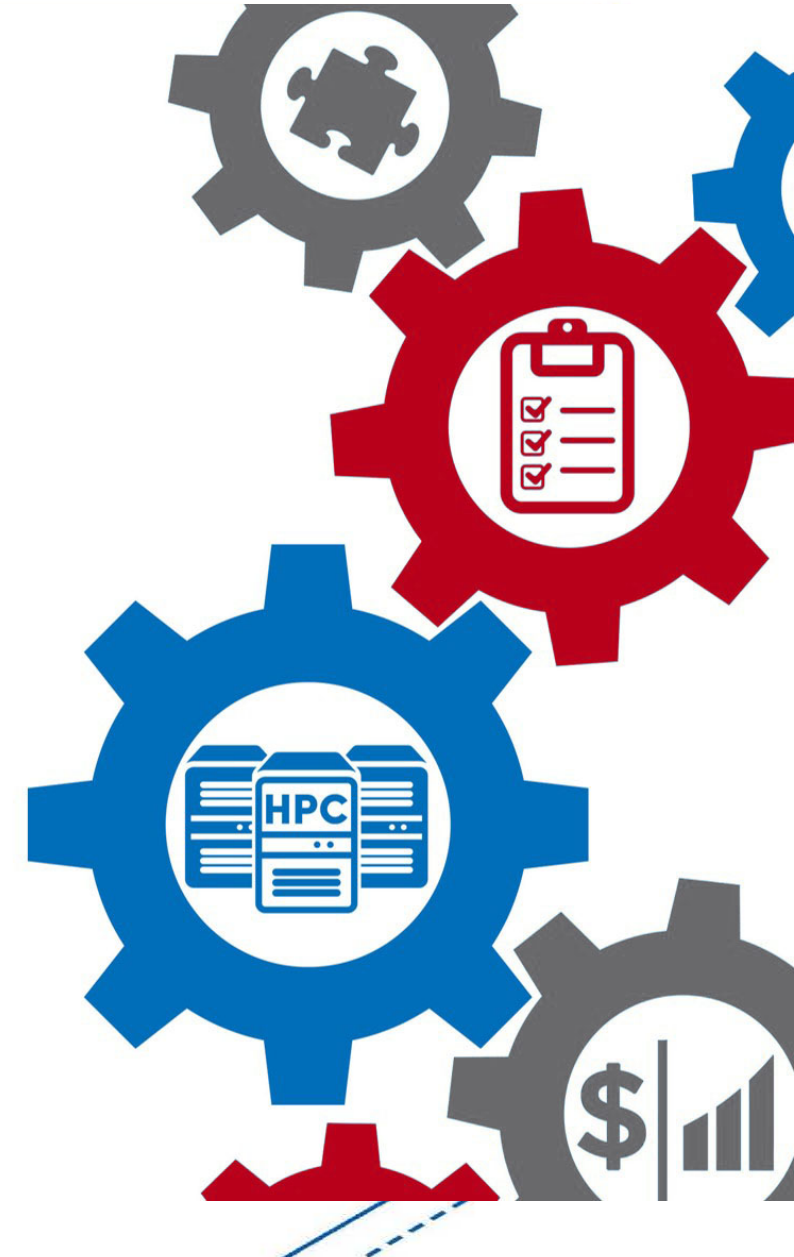






# Tutorial Goals:

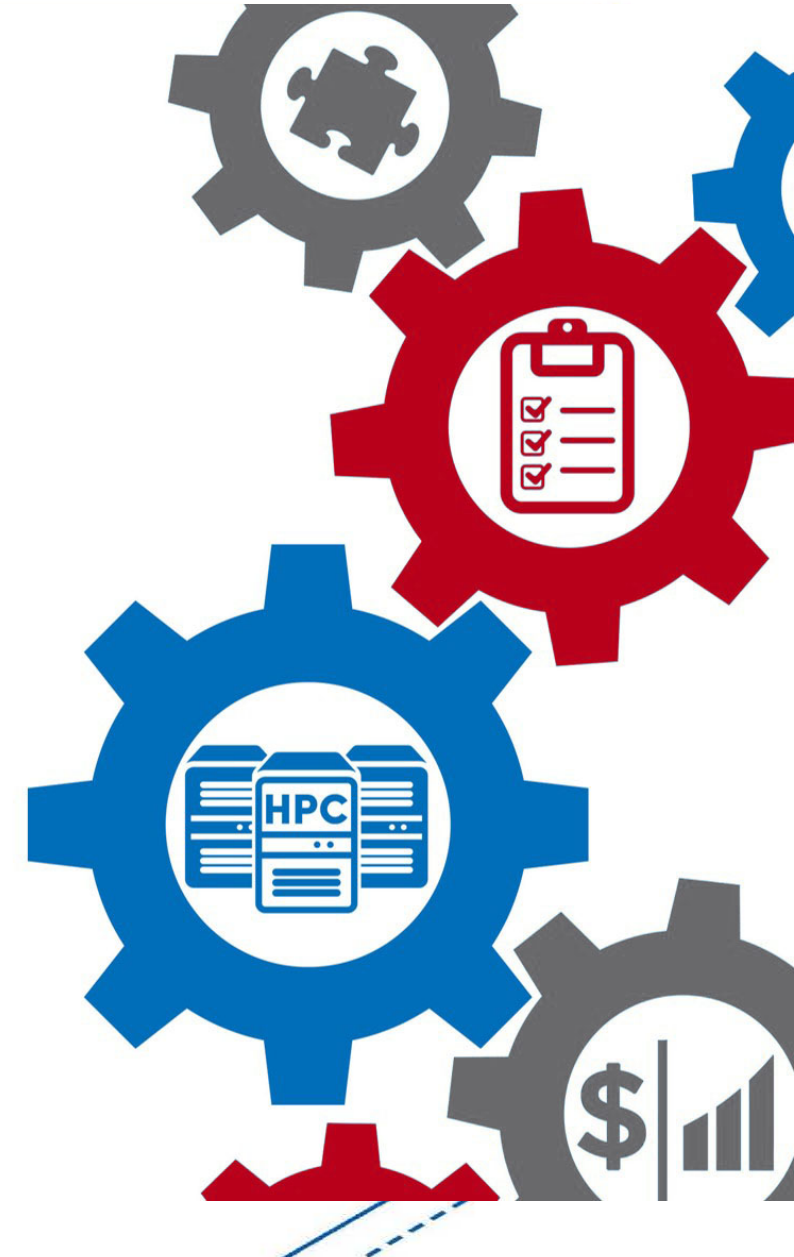
- Provide participants with an overview of each product & how they are installed
- Point out a few “gotcha!”s to look out for
- Give participants a cluster in a container to practice using these products
- Supply participants access to the developers of these products as a resource for questions & help
- Show off the new features that allow the products to work together





## ColdFront – Managing Access

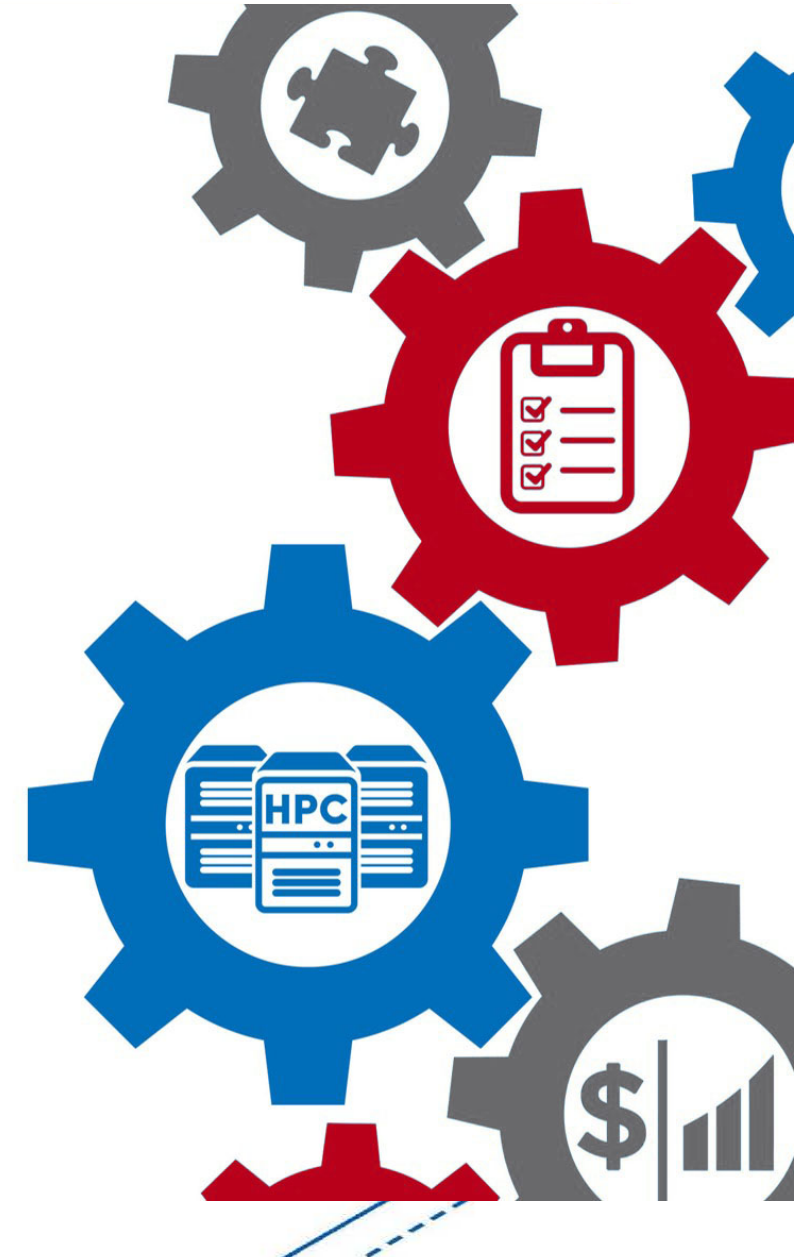
- Used as the source of record in a HPC center to ensure security & continuity of the systems
- Provides center staff ability to manage center resources & who has access to them
- Portal for users to manage their access to center resources & report on their research
- Plug-ins for job scheduler, central authentication, job statistics (XDMoD), OnDemand, that enable automation of access to or removal from resources
- Reports for center management to demonstrate the center's impact (publications, grants, research output)





## Open OnDemand – Easy Access

- Web-based portal for accessing HPC services that removes the complexities of HPC system environments from the end-user. Includes:
- Files app for upload/download & editing of files
- Terminal app (no need for separate SSH client)
- Job app to create/edit/submit/monitor jobs
- Interactive apps to run GUI applications. Users can create and share apps. Centers can publish apps for all users

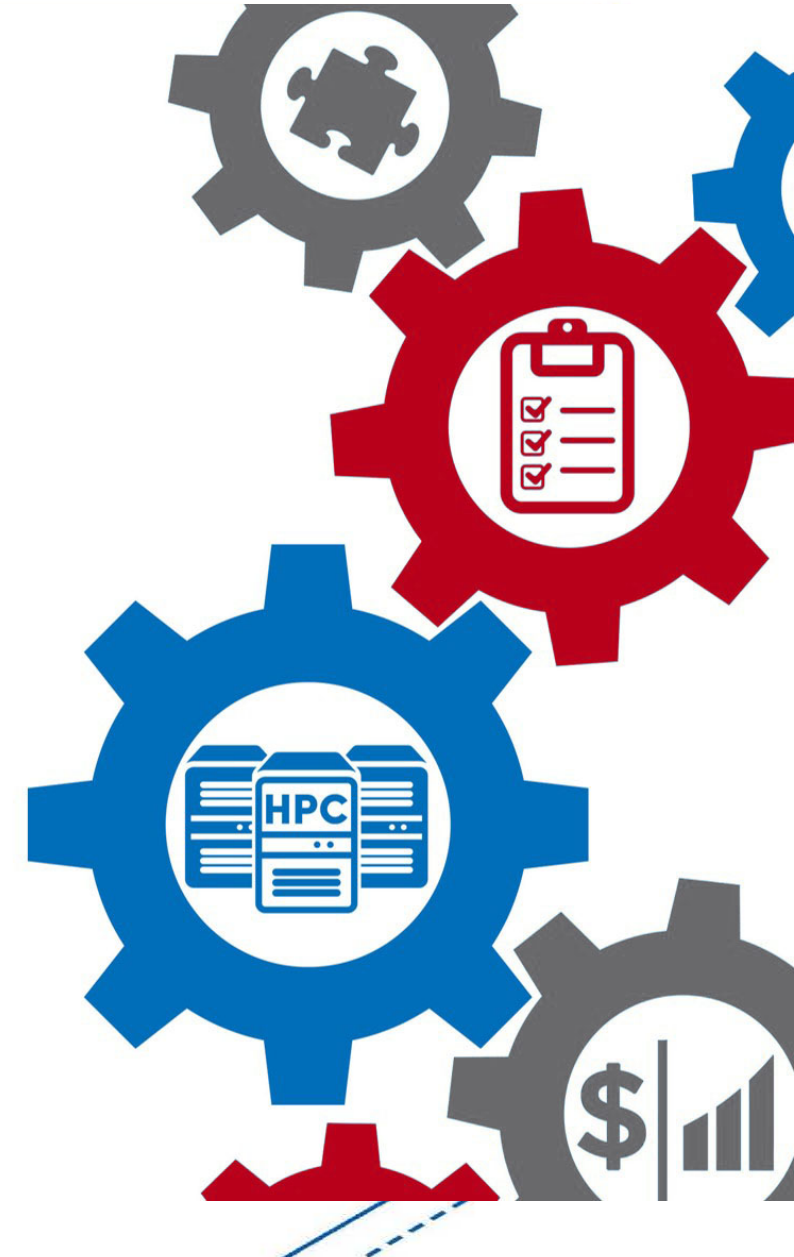






## Open XDMoD – Usage & Performance Metrics

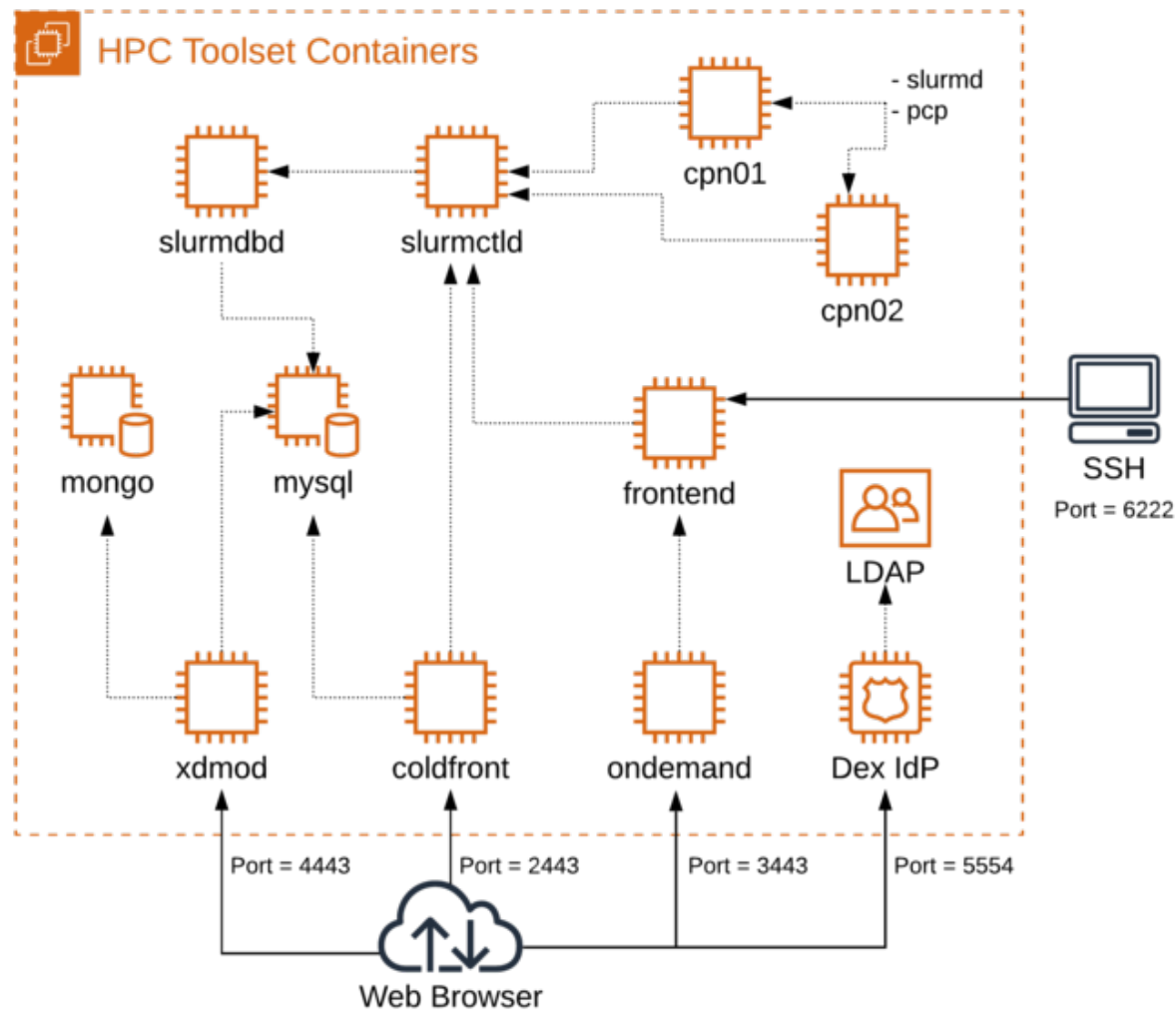
- Tool that aggregates job data & system performance metrics to inform system users, system staff & center decision makers
- Web portal providing job & system metrics, including utilization, quality of service metrics designed to proactively identify underperforming system hardware and software, and job level performance data for every job
- Role-based access to data with different levels of granularity, including job, user, or on a system-wide basis
- Ingest OnDemand logs into new OnDemand realm in XDMoD





# Tutorial Container Architecture

Requirements: <https://github.com/ubccr/hpc-toolset-tutorial/edit/master/docs/requirements.md>



**Clone the Github Repo:**

```
git clone https://github.com/ubccr/hpc-toolset-tutorial
cd hpc-toolset-tutorial
./hpcts start
```

\* The first time you do this, you'll be download ~13GB worth of containers from Docker Hub. This can take a long time depending on your network speeds. After downloaded, the containers are started and services launched.



# Tutorial Walk Through

<https://github.com/ubccr/hpc-toolset-tutorial>

Keep this page open for easy access to account usernames/passwords and portal URLs:

<https://github.com/ubccr/hpc-toolset-tutorial/blob/master/docs/applications.md>



# **ColdFront:** OpenSource HPC resource **allocation portal** for **users, system admins, &** **center staff**

Tutorial presented at PEARC21 by:  
Andrew Bruno, UB  
Dori Sajdak, UB



**Ohio Supercomputer Center**

An **OH·TECH** Consortium Member

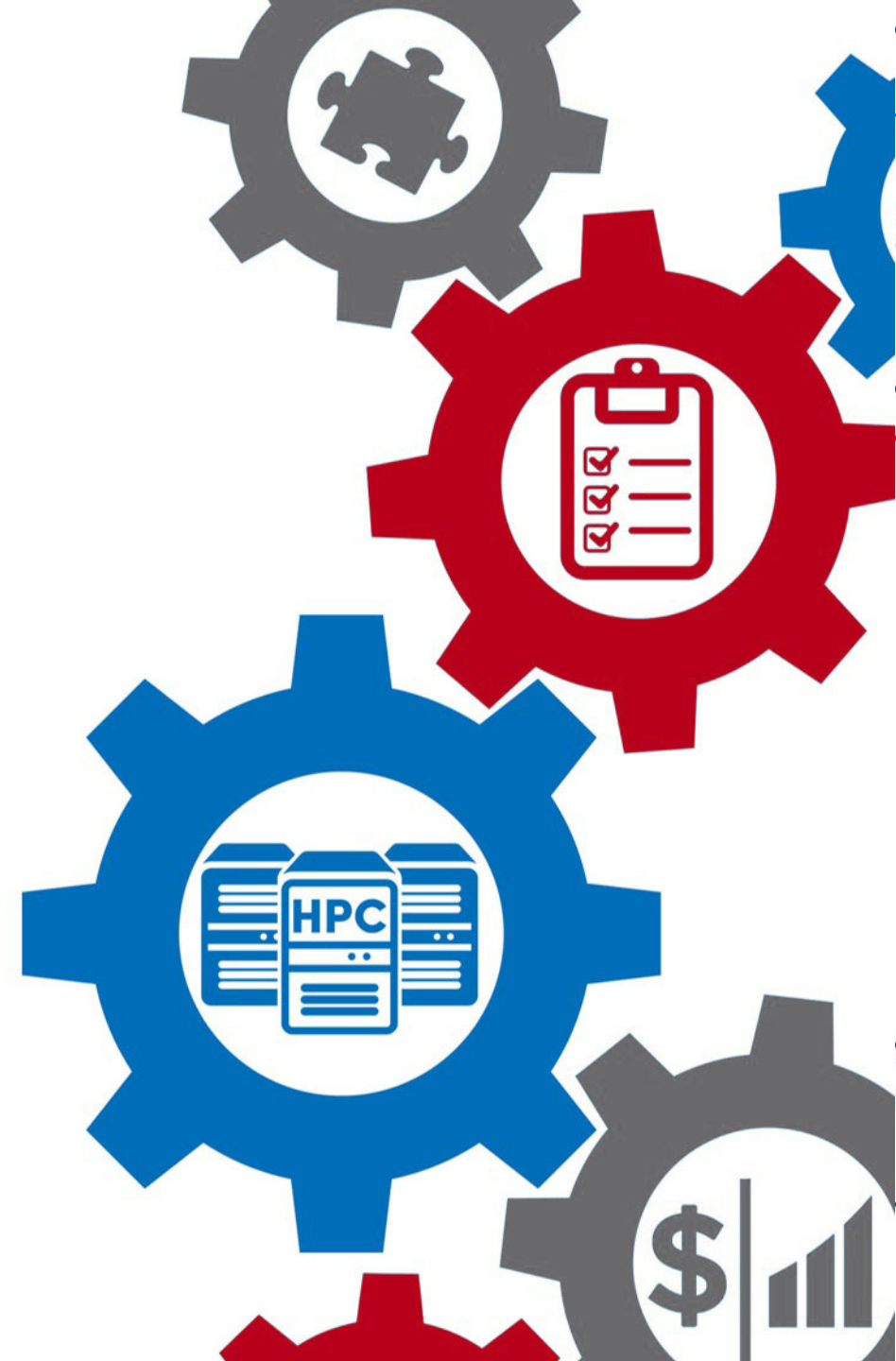


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# Automate access to your HPC resources

Manage access to all your resources in one place

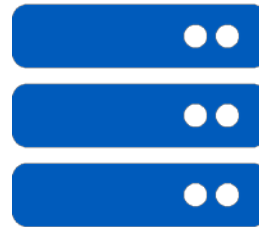


Users



Databases

ACLs



Servers &  
Clusters



Cloud

System  
Administrators

Policies



Software  
Licenses



Storage



Scientific Instruments







## Why We Developed ColdFront:

- System Administrators wanted:
  - More automation, less manual error
  - One location for access management of all resources
  - Allow PIs to self-service access to resources
- Center Director wanted:
  - To require PIs to update project info annually
  - Consistent reporting of publication & grant info
  - Easy displays of usage for annual reporting





## Resources

- Resources are anything you want to control access to and/or monitor usage of
- Resources might include:
  - clusters, storage platforms, cloud, servers, scientific instruments, databases, software licenses
- Some resources have limits:
  - storage (GB),
  - software (seats),
  - cloud (subscriptions)
  - these are all customizable
- Resources can have other attributes that may tie to plugins:
  - Is the resource private or public?
  - Which users/groups are allowed access to it
  - Is payment required?
  - Warranty expiration dates





## Allocations

- Determines what resource an account has access to
- Any limits/attributes associated with that access
  - Expiration date
  - CPU/core hours
  - Scheduler account name
  - UNIX group
  - Storage quota
- Users emailed when expiration dates approach
- Resource access can be removed/locked when an allocation expires





## Projects

- Project = users, allocations for resources, reportable data (publications, grants)
- PIs (group leads) can request allocations for resources, add/remove users on their project & allocations, upload research info, complete annual project review, view group usage
- Role based logins allow for:
  - full project access for PIs
  - additional capabilities for managers assigned by PIs,
  - read-only views for users,
  - HPC center staff have access to tools for:
    - Allocation review, approval, & configuration
    - Annual project review approval
    - Other policy-driven tools





# Annual Project Reviews Completed by PIs Can be Viewed by Center Director and System Administrators

## Pending Project Reviews

Project Title	Date Review Submitted	PI	Grants Last Updated	Publications Last Updated	Reason for not Updating Project	Project Review Actions
<a href="#">My Test Project</a>	May. 13, 2021	Dori Sajdak (djm29)	May. 13, 2021	May. 13, 2021		<a href="#">Mark Complete</a> <a href="#">Email</a>

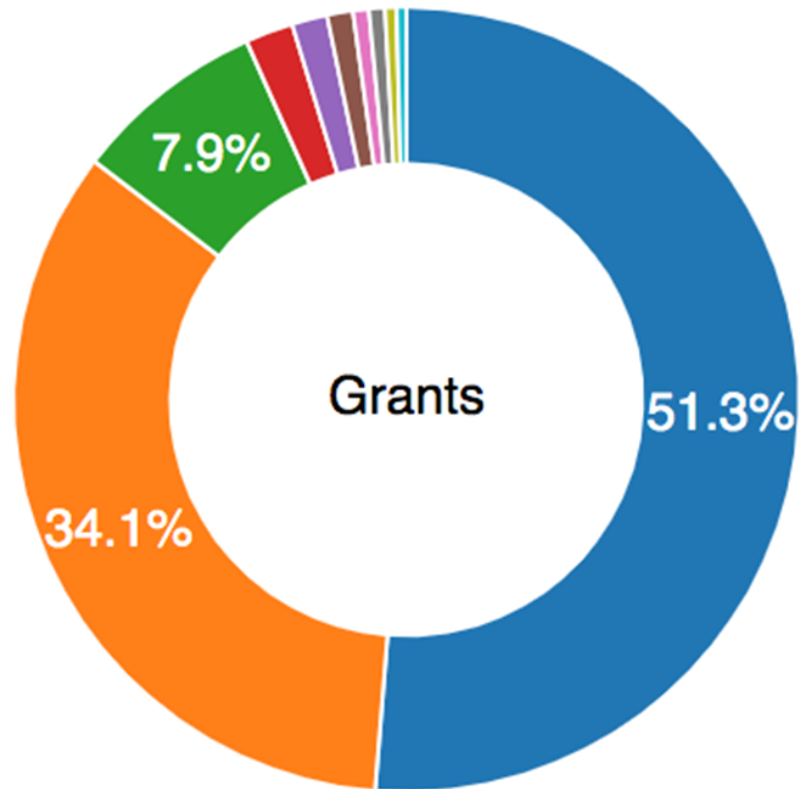
## Allocation Requests

# Allocation Requests Can be Viewed by System Administrators

#	Date Requested/ Last Modified	Project Title	PI	Resource	Project Review Status	Status	Allocation Actions
825	Apr. 08, 2021	<a href="#">Interplay Between Genetics and Epigenetic in Poly...</a>	James Jarvis (jamesjar)	ProjectStorage (Storage)		Renewal Requested	<a href="#">Activate</a> <a href="#">Deny</a>
838	Apr. 30, 2021	<a href="#">Hachmann Group Research</a>	Johannes Hachmann (hachmann)	ProjectStorage (Storage)		Renewal Requested	<a href="#">Activate</a> <a href="#">Deny</a>
845	Apr. 01, 2021	<a href="#">Wilson Lab</a>	Adam Wilson (adamw)	ProjectStorage (Storage)		Renewal Requested	<a href="#">Activate</a> <a href="#">Deny</a>
1874	Apr. 01, 2021	<a href="#">Samudrala Computational Biology Research Group</a>	Vaikuntanath Samudrala (rams)	ProjectStorage (Storage)		Renewal Requested	<a href="#">Activate</a> <a href="#">Deny</a>
2079	May. 13, 2021	<a href="#">My Test Project</a>	Dori Sajdak (djm29)	UB-HPC Academic (Cluster)		Renewal Requested	<a href="#">Activate</a> <a href="#">Deny</a>







■ National Institutes of Health (NIH): \$78,599,277 (33)  
■ National Science Foundation (NSF): \$52,283,068 (73)  
■ Other: \$12,161,778 (49)

Center Directors are able to better demonstrate the center's impact

**Report on resources & allocations**

**Collect publication information**

**Collect grant information**





# Extensible plug-in architecture allows for **integration of nearly anything!**



Vendor APIs





## Integrations

Plug-ins (Django Apps)

- [OnDemand](#)
- [XDMoD](#)
- [Slurm](#)
- [Mokey/Hydra OpenID Connect](#) (Identity Management)
- [FreeIPA](#) (LDAP/AD)
- [Other plug-in examples](#)
- Other 3<sup>rd</sup> party APIs should be added as a new plug-in (Django app)
- In the works – OpenStack plug-in





## Tutorial Steps:

- Create different user roles and access
- Create new cluster resource
- As PI user, create project and request allocation for cluster resource
- As sys admin user, activate allocation and sync with Slurm
- As PI user, run batch & OnDemand job
- Ingest job data into XDMoD and view as PI user
- Enable OnDemand integration
- Configure user with staff access
- Check out Project Review process (time permitting)



## Contact Info:

[Andrew Bruno - aebruno2@buffalo.edu](mailto:aebruno2@buffalo.edu)

[Dori Sajdak - djm29@buffalo.edu](mailto:djm29@buffalo.edu)

<https://coldfront.io>

Subscribe to the ColdFront mailing list:

Send an email to [listserv@listserv.buffalo.edu](mailto:listserv@listserv.buffalo.edu) with no subject, and the following command in the body of the message:

```
subscribe ccr-open-coldfront-list@listserv.buffalo.edu first_name last_name
```

More about UB CCR:

<https://buffalo.edu/ccr>

<https://twitter.com/ubccr>

ColdFront Use Cases BOF:  
Tues, 7/20 11:15am-12:15pm PST  
Panel of presenters from Harvard, USC, and Virginia Tech discuss how they're using CF

ColdFront short paper presentation:  
Thurs, 7/22 8:15-8:25am PST



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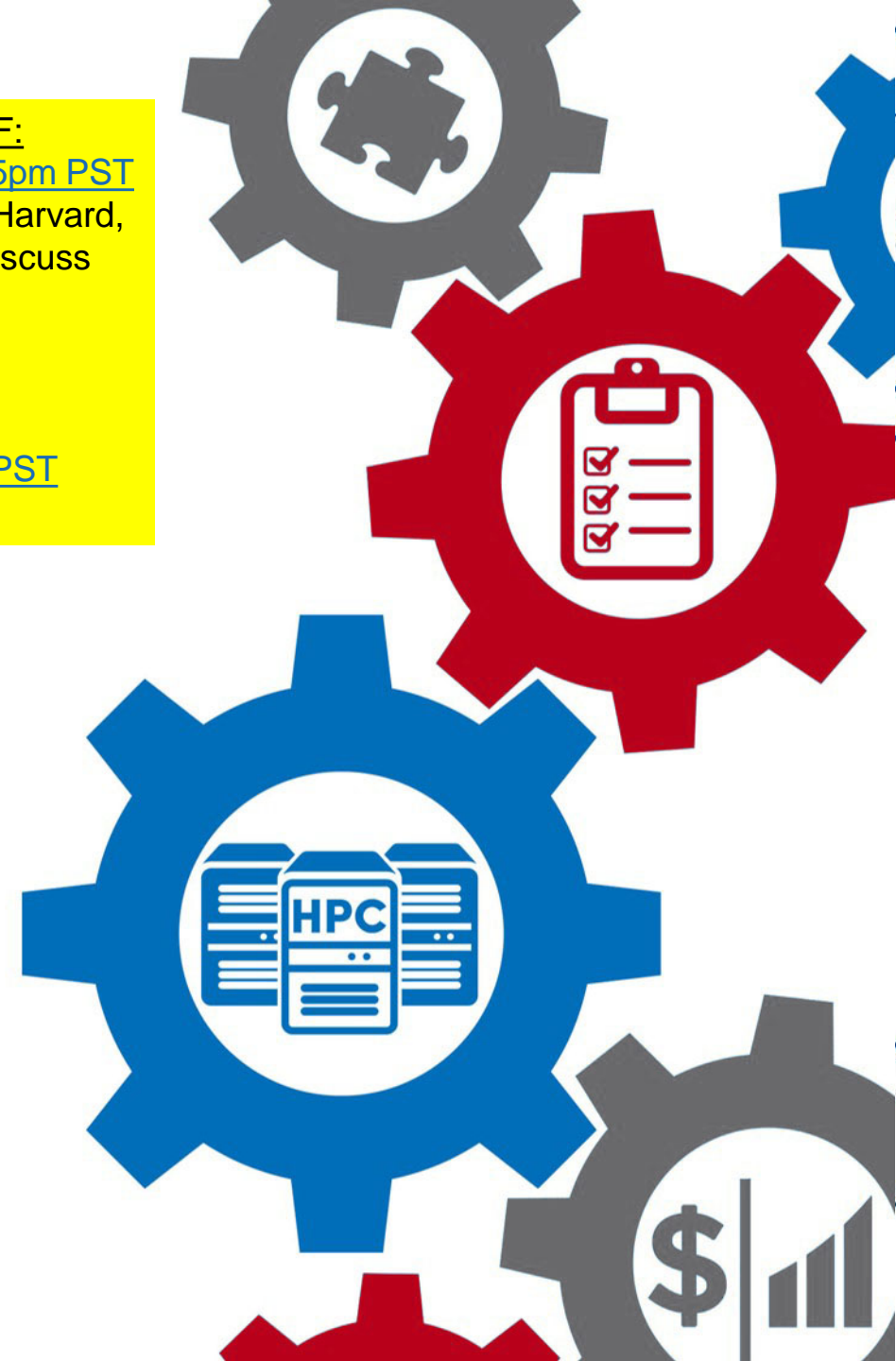


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A photograph of a server room with blue lighting. In the center, a man and a woman are standing and talking. The man is holding a tablet. The room is filled with server racks on both sides, and the floor is a blue grid. The ceiling has recessed lighting and ventilation ducts.

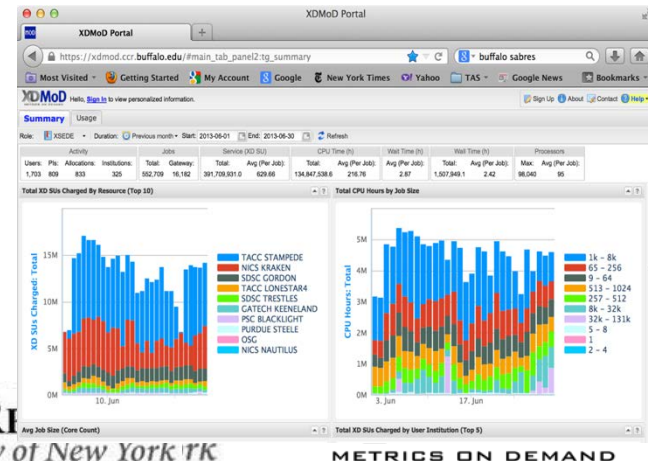
# Introduction to XDMoD

Center for Computational Research  
University at Buffalo, SUNY  
PEARC21 July 2021

# XDMoD: A Comprehensive Tool for HPC System Management

- **XD Net Metrics Service (XMS) NSF Award to CCR**
  - Following 5 year TAS award on-going 6-year XMS award
  - Develop **XDMoD (XD Metrics on Demand) Tool**
- **XSEDE XDMoD**
- **Open XDMoD: Open Source version for Data Centers**
  - 400+ academic & industrial installations worldwide
- **Goal: Optimize Resource Utilization and Performance**
  - Provide instantaneous and historical information on utilization
  - Measure Quality of Service
  - Enable data driven upgrades and procurements
  - Measure and improve job and system level performance

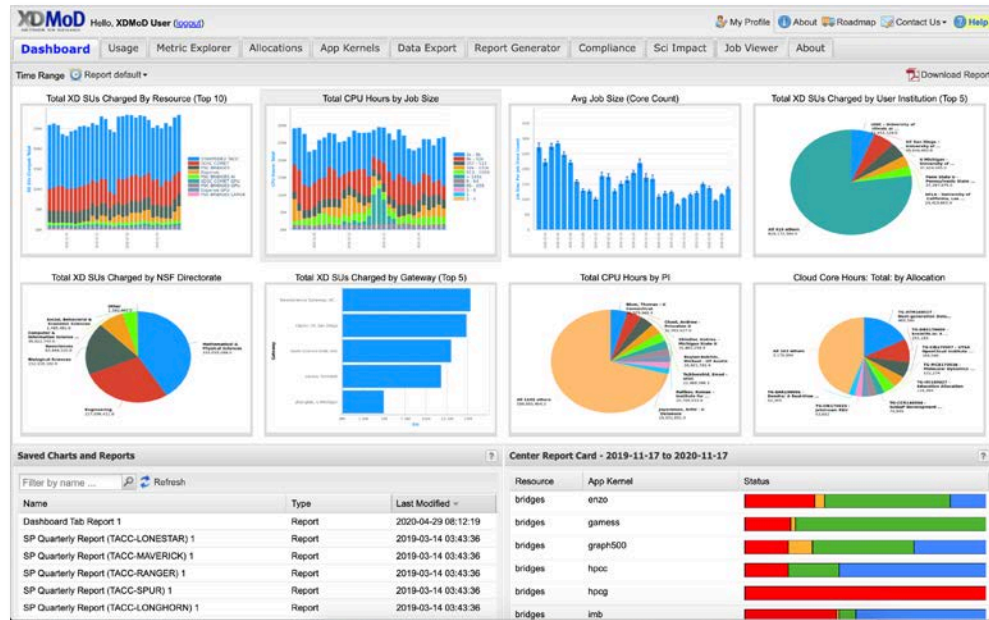
**XDMoD**  
METRICS ON DEMAND





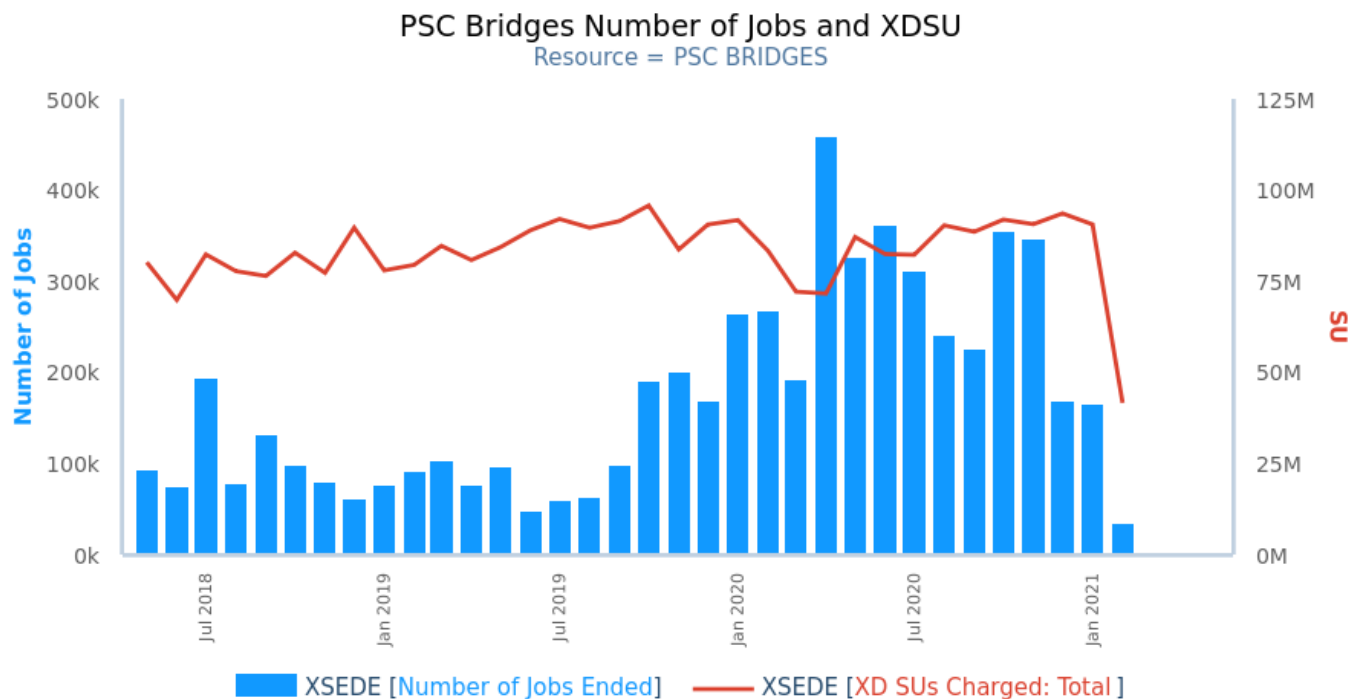
# Primary Components of XDMoD

- XDMoD web Portal
  - Metrics Explorer for reports on system usage and efficiency
  - Job Viewer to Measure and improve job performance
- Application Kernels
  - Measure Quality of Service



# XDMoD Portal

- Web-based
- Display metrics
  - Job accounting data and job performance data (supremm)
- Scientific impact
- Custom Report Generator
- Role based access

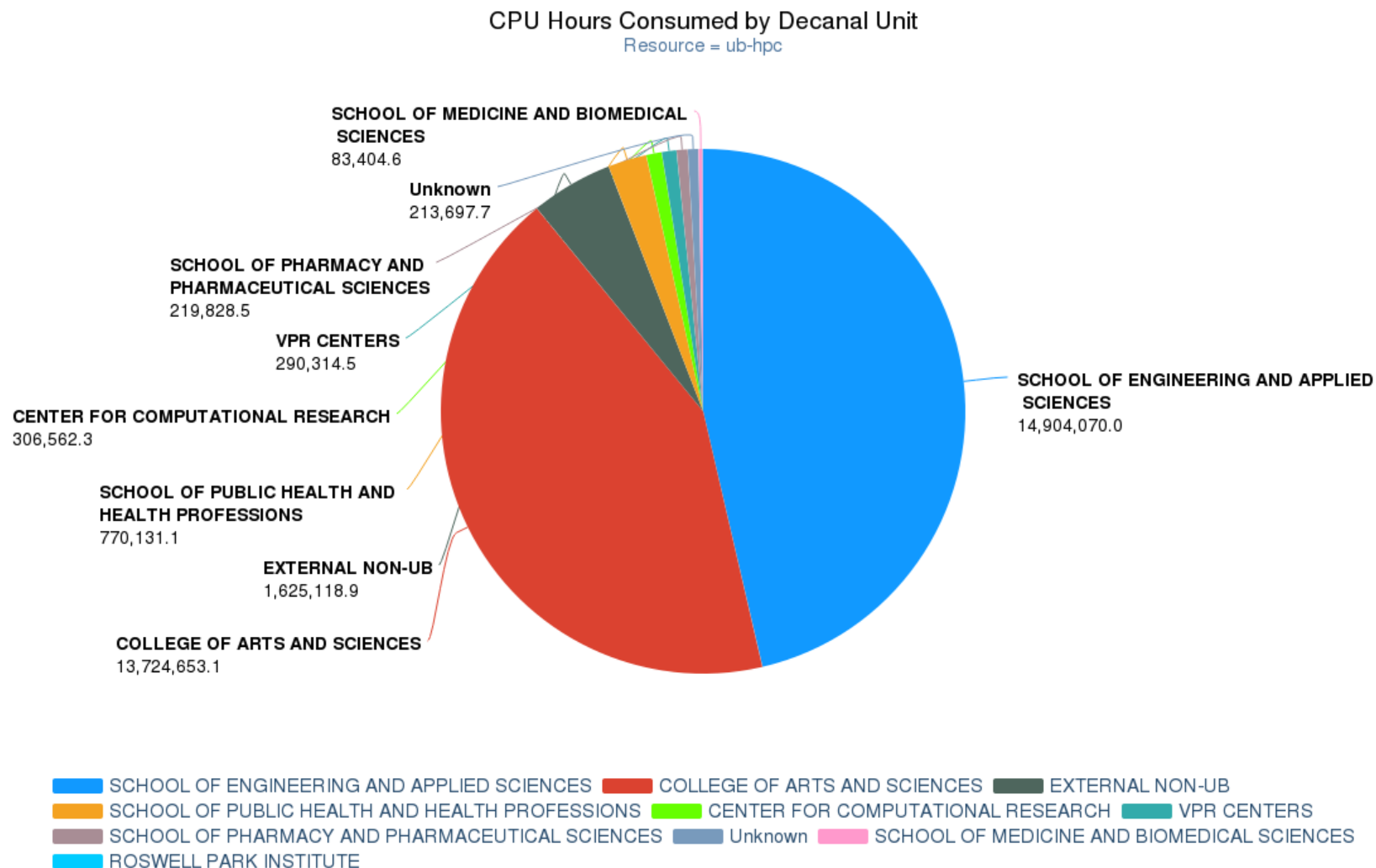


2018-05-01 to 2021-05-11 Src: XDCDB. Powered by XDMoD/Highcharts



# Easily Obtain Utilization Metrics

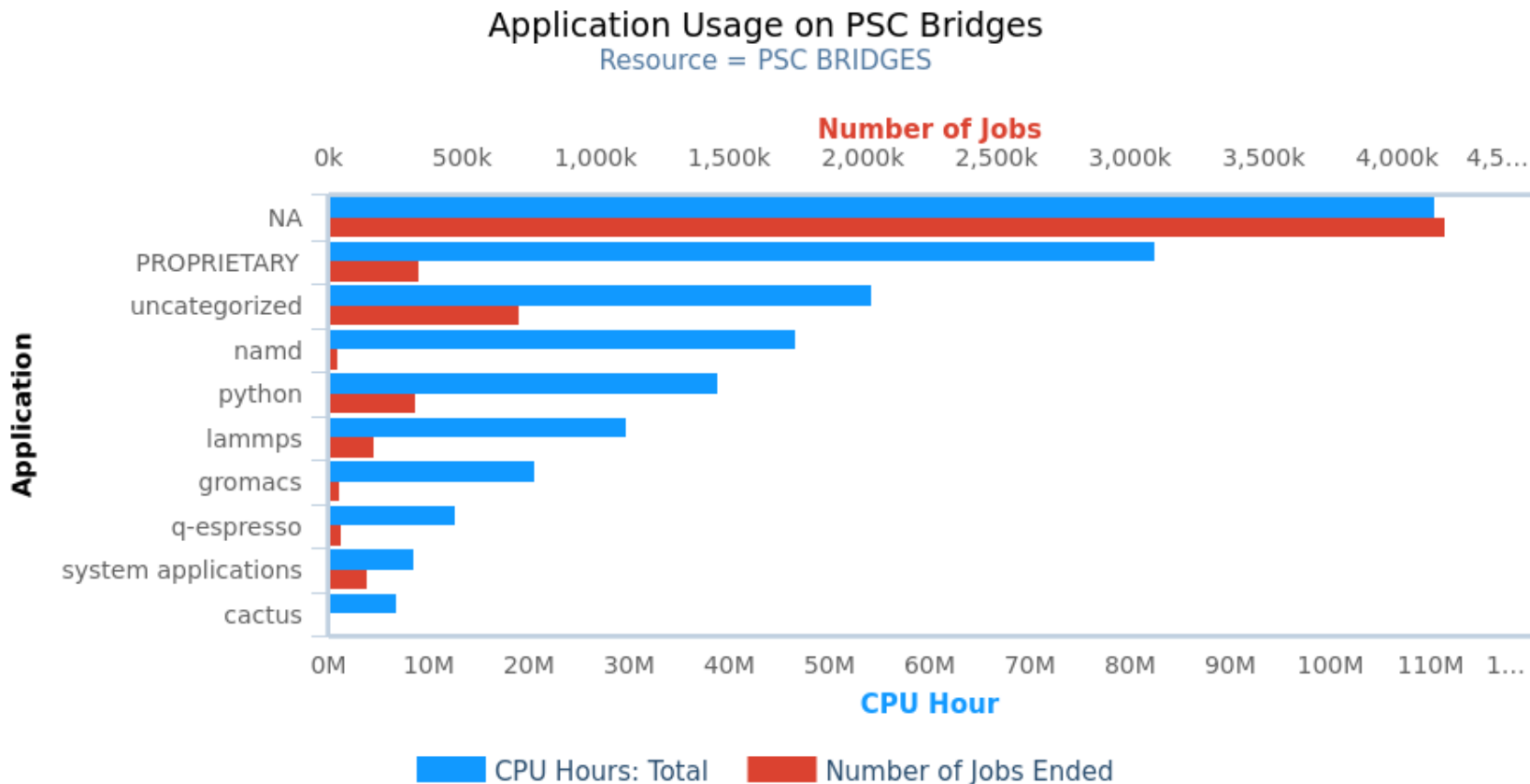
- CPU hours consumed by campus units





# Uses: Application Analysis

- Determine what are the mostly widely used applications running on PSC Bridges for the last 3 years

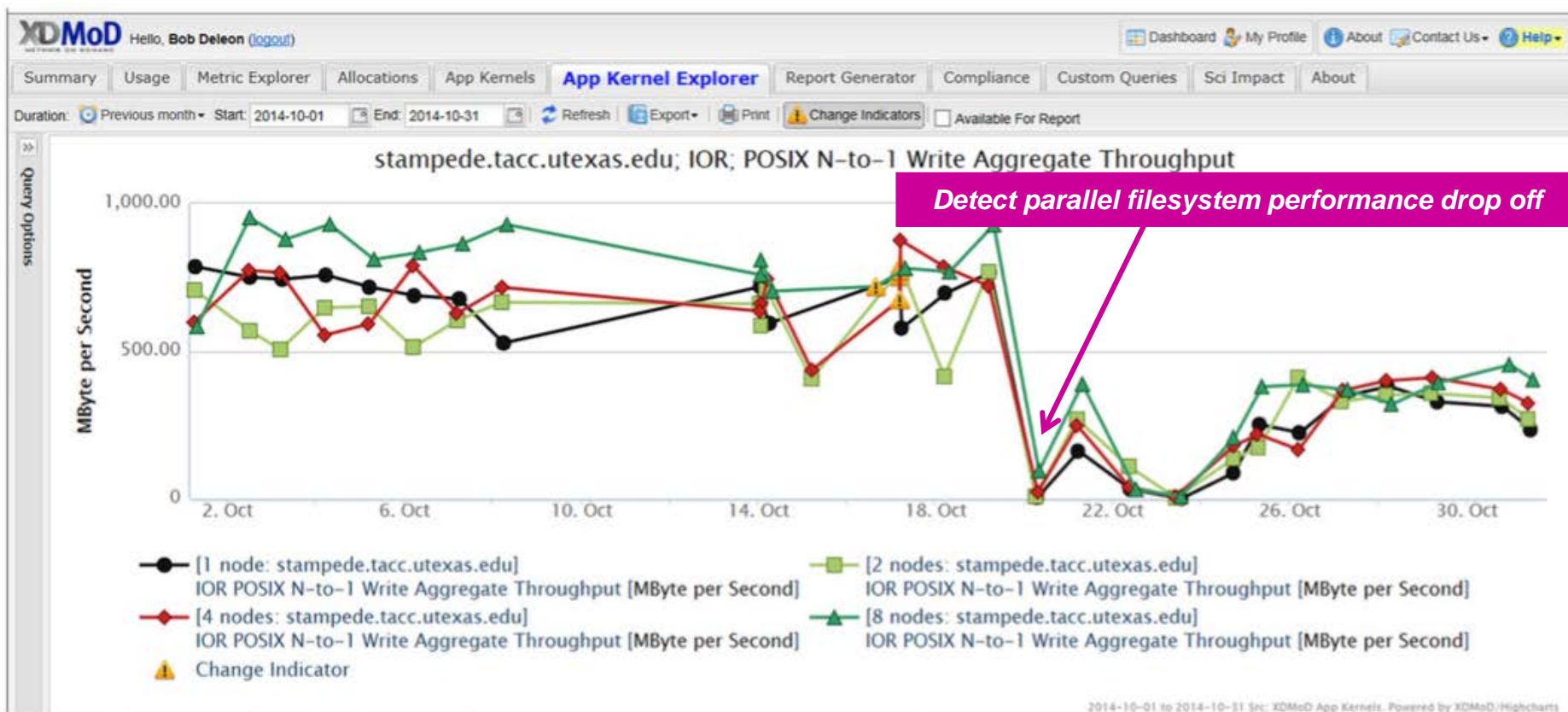


2018-05-01 to 2021-05-11 Src: SUPREMM. Powered by XDMoD/Highcharts

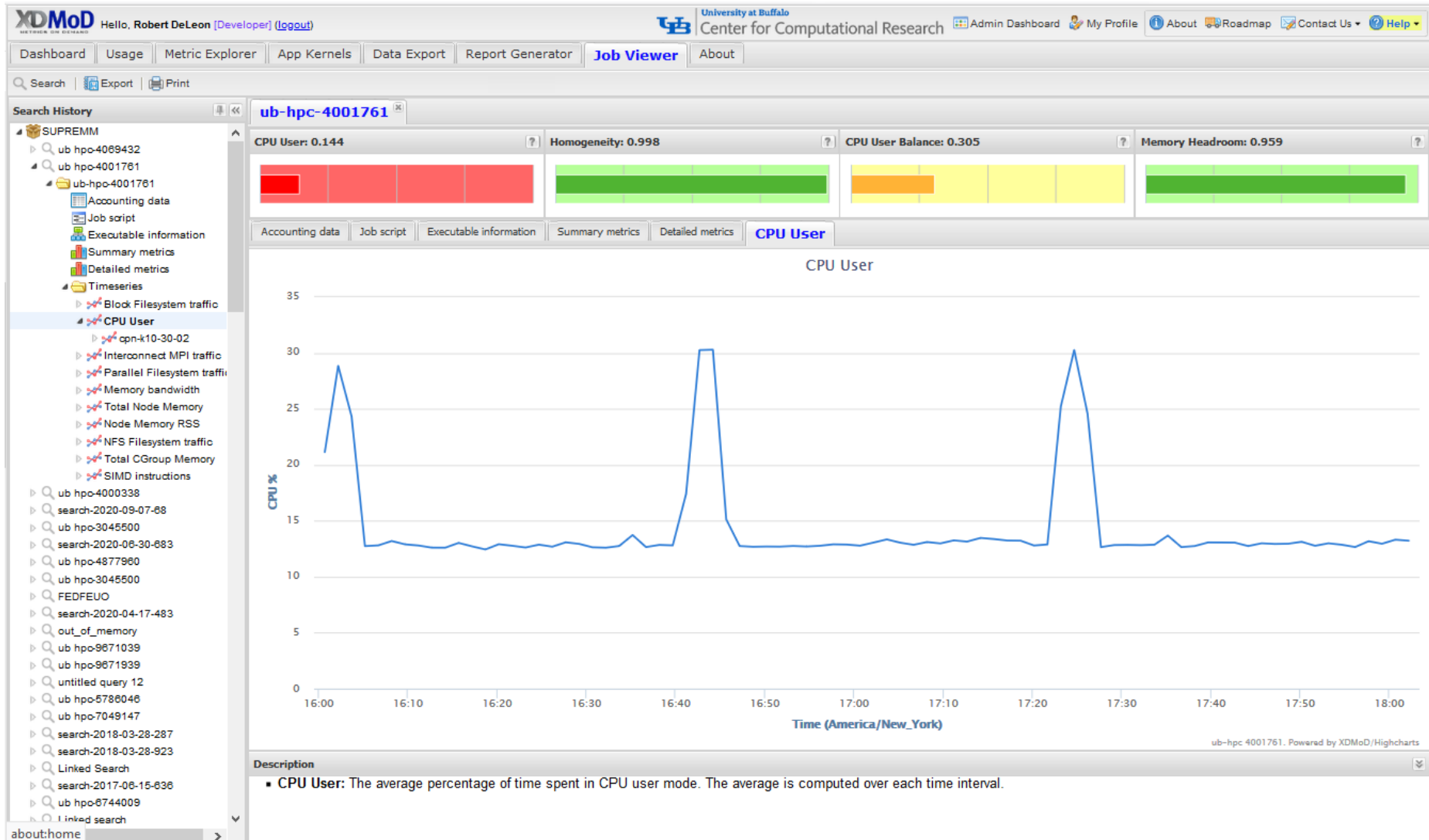


# QoS: Application Kernels

- Computationally lightweight benchmarks or applications
  - Run periodically or on demand to actively measure performance
- Measure system performance from User's perspective
  - Local scratch, global filesystem performance, local processor-memory bandwidth, allocatable shared memory, processing speed, network latency and bandwidth
- Proactively identify underperforming hardware and software



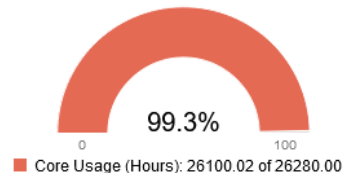
# Job Viewer: Measuring Job Performance



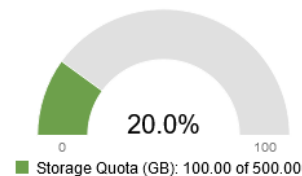
# ColdFront Integration

- CF uses the XDMoD API to obtain Core Usage and Storage Information for cloud accounts

Core Usage (Hours)



Storage Quota (GB)





# XDMoD OnDemand Integration

- Open OnDemand: “one stop shop for quick access to HPC”
  - OSC (Dave Hudak PI) & CCR (Tom Furlani coPI)
- Key program goal to integrate XDMoD into Open OnDemand.

The screenshot displays the Ohio Supercomputer Center (OSC) OnDemand dashboard. The page features a navigation bar with links for Files, Jobs, Clusters, Interactive Apps, My Interactive Sessions, and All Apps. The main content area includes a 'Message of the Day' section with news about COVID-19 support and distance learning. On the right, there are three XDMoD efficiency reports and a job list table.

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OnDemand provides an integrated, single access point for all of your HPC resources.

### Message of the Day

**2020-03-16 - OSC support during COVID-19 crisis**

The Ohio Supercomputer Center serves as a critical resource for the public good and, as such, is striving to provide extraordinary support in light of the ongoing COVID-19 crisis. OSC staff are currently working from home but fully expect clients will see no disruption in our services to support this effort.

Examples of the types of special support OSC can provide include: - Priority, unbilled access to OSC computational and storage resources for COVID-19 research - Flexible billing terms and prices for clients anticipating negative economic impacts - Remote, virtual computing lab resources for classroom instructors and educators - Connections to domain experts in academia and industry

Please don't hesitate to contact OSC at [oschelp@osc.edu](mailto:oschelp@osc.edu) or (800) 686-6472 for more information on this initiative. Please also distribute this message via any communication channel you to which you might have access so that it can be distributed as widely as possible.

**CLASSROOM RESOURCES FOR DISTANCE LEARNING**

If your class has lost or limited access to computer labs, the Ohio Supercomputer Center might be able to help by providing no-cost access to cloud computing resources. Classes and workloads of any size can gain access. OSC's web-browser interface to its substantial Linux computer systems provides novice users with virtual desktops preloaded with applications, such as MATLAB, RStudio, or Jupyter Notebook.

As an example, an OSU undergrad statistics class recently used iPads to remotely access RStudio on OSC systems. We can provide online demonstrations or evaluations and potentially add additional software packages.

Please contact [OSCHelp@osc.edu](mailto:OSCHelp@osc.edu) to talk to OSC about distance-learning support options available to you.

**2020-03-09 - Huge memory nodes partial scheduling**

Beginning on Tuesday, March 10th users are able to run jobs using less than a full huge memory node on both the Owens and Pitzer clusters.

Please consider your request more carefully when you plan to use a huge memory node, and specify the resources based on what you will use. Please check our documentation for more detailed guidance: [https://www.osc.edu/resources/technical\\_support/supercomputers/owens/batch\\_limit\\_rules](https://www.osc.edu/resources/technical_support/supercomputers/owens/batch_limit_rules) [https://www.osc.edu/resources/technical\\_support/supercomputers/pitzer/batch\\_limit\\_rules](https://www.osc.edu/resources/technical_support/supercomputers/pitzer/batch_limit_rules)

**2019-10-03 - Wall-time Accuracy Information**

Due to current usage patterns on OSC's Owens Cluster, users may benefit from improving the wall-time accuracy of their submitted jobs. A job has high wall-time accuracy if the requested wall time comes near the actual wall time when the job completes.

The benefit of improving one's wall-time accuracy is that the requested wall time is taken into account when scheduling jobs to run. Usually, jobs that request shorter wall time, ceteris paribus, will wait for less time than jobs requesting longer wall times. One can investigate the accuracy of their previous jobs using the following HOW TO webpage: [https://www.osc.edu/resources/getting\\_started/howto/how\\_to\\_look\\_at\\_wall\\_time\\_accuracy\\_using\\_xdm](https://www.osc.edu/resources/getting_started/howto/how_to_look_at_wall_time_accuracy_using_xdm)

Contact OSC Help if you questions, comments or concerns

### XDMoD - Job Efficiency Report - 2020-05-27 to 2020-06-26

44.1% efficient 55.9% inefficient

33 inefficient jobs / 59 total jobs

### XDMoD - Core Hours Efficiency Report - 2020-05-21 to 2020-06-20

71.2% efficient 28.8% inefficient

580.2 inefficient core hours / 2013.0 total core hours

### XDMoD - Jobs - 2020-05-27 to 2020-06-26

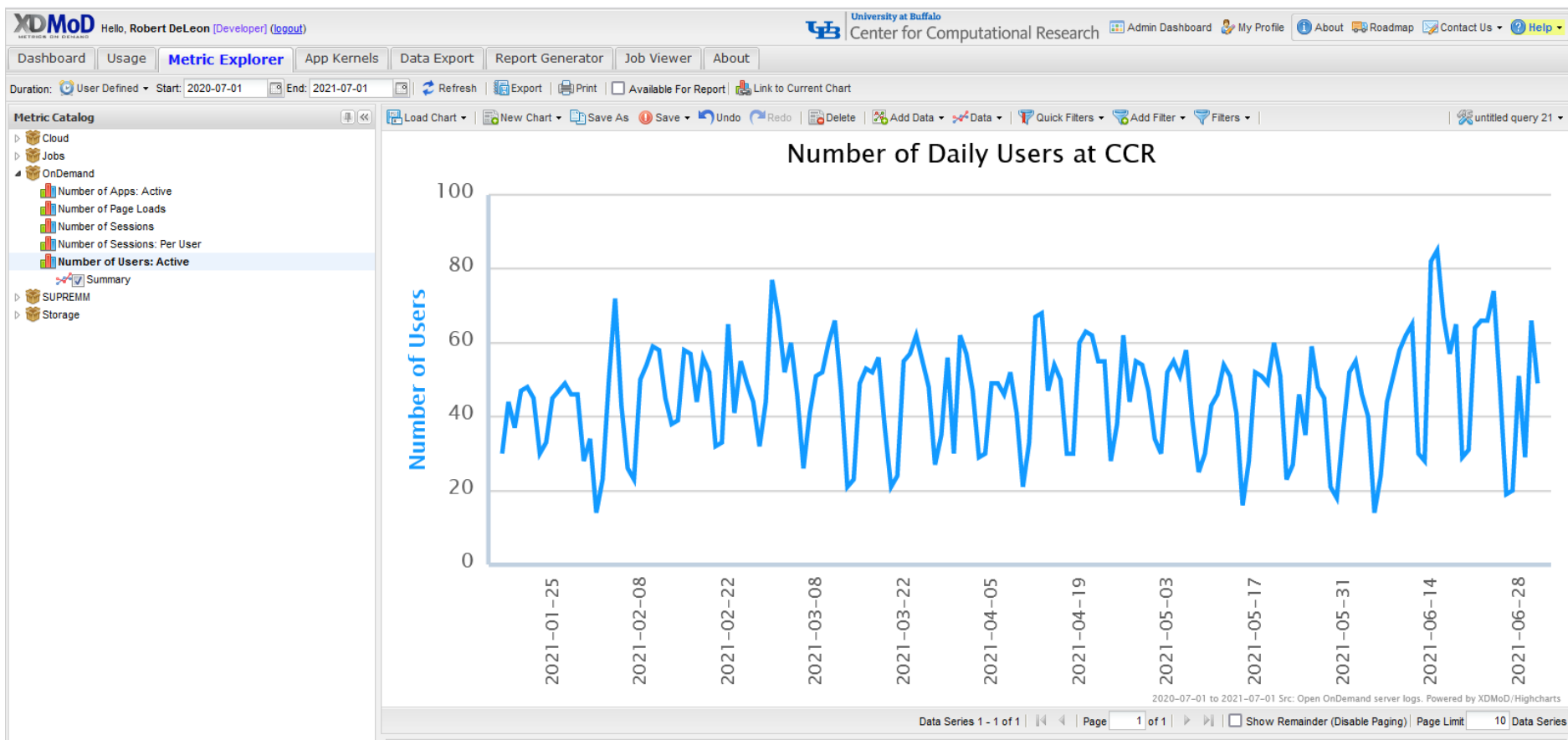
ID	Cluster	Date	Time Used	CPU
10573480	owens	6/5	00:14:00	86.3
10573479	owens	6/5	00:02:08	28.7
10573468	owens	6/5	00:04:40	91.4
10572847	owens	6/5	00:30:55	00.8
10572013	owens	6/5	00:31:27	06.0
10572010	owens	6/5	00:00:03	N/A
10572007	owens	6/5	00:00:04	N/A
10539927	owens	6/1	02:00:41	06.1
10539673	owens	6/1	00:17:23	10.5
10539512	owens	6/1	00:44:25	09.9

Showing first 10 of 58 jobs. See your XDMoD dashboard for more information.



# XDMoD Realm for OnDemand Usage

- XDMoD can also provide usage information to OnDemand providers.





- XDMoD and Starfish are exploring integration possibilities.
- Starfish is a commercial software product that combines a data catalog for unstructured data with a high-performance batch processor and data mover.
- XDMoD can tap the Starfish database through API or native SQL, providing much richer storage insights, especially on large, complex file systems.
- Starfish's catalog integrates with HPC file systems and scale-out NAS to support billions of files.
- Starfish's catalog supports tagging (on files and directories) as well as key-value metadata.
- We welcome your participation:
  - Starfish will provide a **no-cost collaborator's license** to PEARC member organizations that are not Starfish customers and want to join in the effort.
  - Contact: [sales@starfishstorage.com](mailto:sales@starfishstorage.com).



# XMS Team

- **XD Metrics Service (XMS)**

- **CCR:** Tom Furlani, Matt Jones, Bob DeLeon, Joe White, Jeff Palmer, Nikolay Simakov, Jeanette Sperhac, Ryan Rathsam, Gregory Dean, Hannah Taylor, Cynthia Cornelius, Abani Patra
- **Indiana:** Gregor von Laszewski, Fugang Wang
- **TACC:** Bill Barth, Todd Evans

- **Former TAS/XMS**

- Amin Ghadersohi, Steven Gallo, Ben Plessinger, Martins Innus, Ryan Gentner, Thomas Yearke, Charng-Da Lu, James Browne, Rudra Chakraborty

- **NSF**

- TAS: OCI I025159, SUPReMM: OCII203560
- XMS: ACI-I445806,



# Contact Information

- XSEDE XDMoD
  - <https://xdmod.ccr.buffalo.edu/>
- Open XDMoD
  - <https://open.xdmod.org/>
- XDMoD Help
  - [ccr-xdmod-help@buffalo.edu](mailto:ccr-xdmod-help@buffalo.edu)
- XDMoD/Open XDMoD Mailing List
  - <https://listserv.buffalo.edu/cgi-bin/wa?SUBED1=ccr-xdmod-list&A=I>







<https://www.osc.edu/> <https://openondemand.org/>

OnDemand team is hiring: <https://go.osu.edu/ood-job>

<https://buffalo.edu/ccr>

<https://open.xdmod.org/>

<https://coldfront.io>

<https://arc.vt.edu/>

## Important Info:

Tutorial Repo: <https://github.com/ubccr/hpc-toolset-tutorial>

Decorum Doc: <https://tinyurl.com/pearc-hpctoolset>

Join us on Slack: <https://tinyurl.com/pearc-slack>

**IF YOU HAVE NOT ALREADY DONE SO,  
PLEASE FOLLOW SETUP INSTRUCTIONS!**

**NOW: Break: 30 minutes – Start up again at  
12:20 PDT / 3:20 EDT**

### Coming Up!

Part 3: Open OnDemand install & configuration

Part 4: Open OnDemand interactive app configuration

Break: 15 minutes

Part 5: Open OnDemand & Open XDMoD integration

Post Workshop – breakout sessions

## Other Places You'll Find us at PEARC21:

Open OnDemand User Group Meeting: Tues, 7/20 11:15am **PST**

ColdFront Use Cases Panel BOF: Tues, 7/20 11:15am

Ookami Deployment & Initial Experiences: Wed, 7/21 10am

ColdFront short paper presentation: Thurs, 7/22 8:10am

**Please answer the Polls  
under the workshop in  
Pathable if you haven't  
already. Thanks!**



**OPEN**

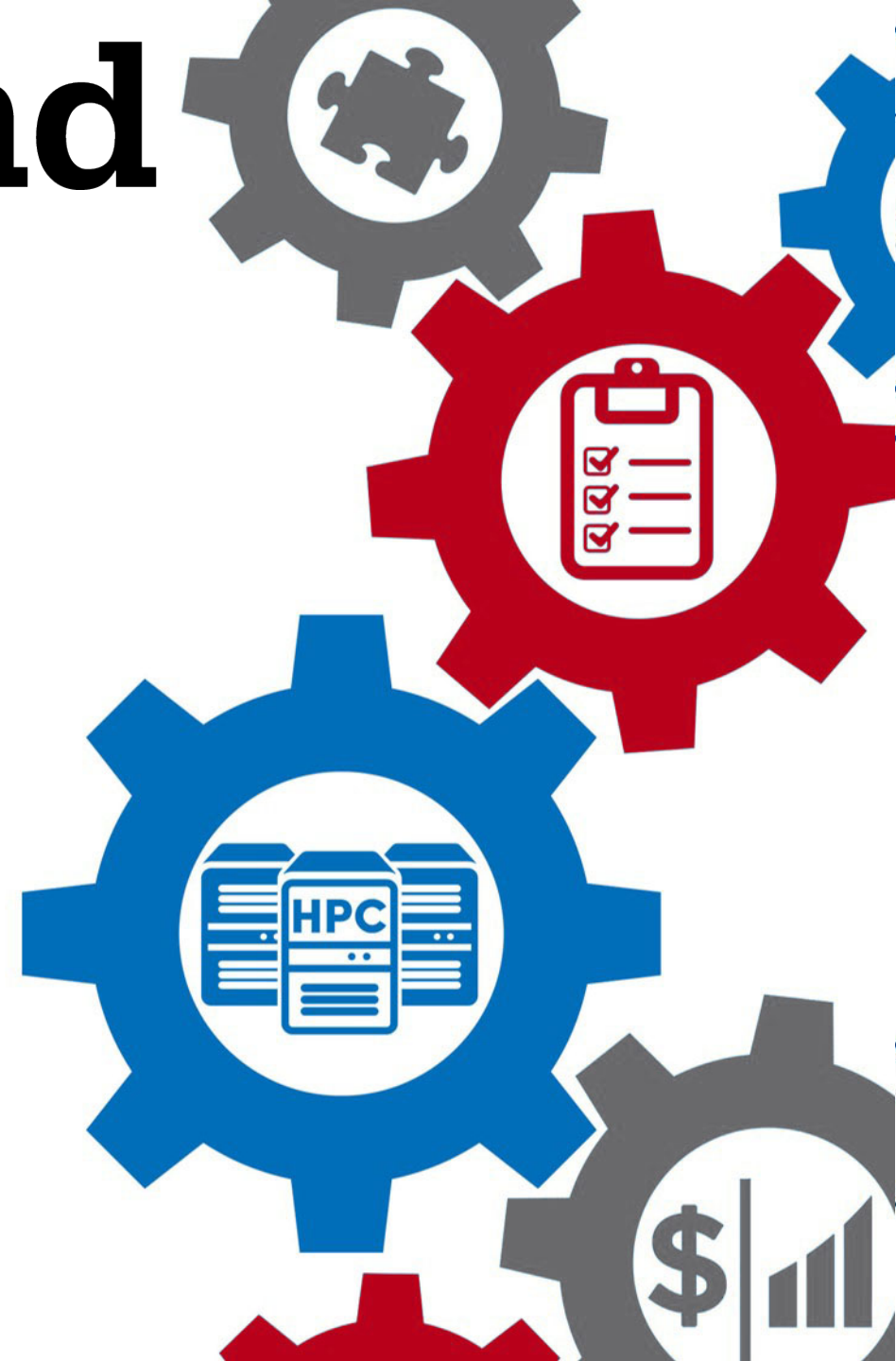
# **nDemand**

## Open, Interactive HPC via the Web

Alan Chalker, OSC  
Travis Ravert, OSC  
Trey Dockendorf, OSC  
Jeff Ohrstrom, OSC  
Bob Settlage, VT

OSC has a job opening on the Open OnDemand team!

Full details are available here:  
[go.osu.edu/ood-job](http://go.osu.edu/ood-job)



**Ohio Supercomputer Center**  
An OH·TECH Consortium Member



 **University at Buffalo**  
Center for Computational Research

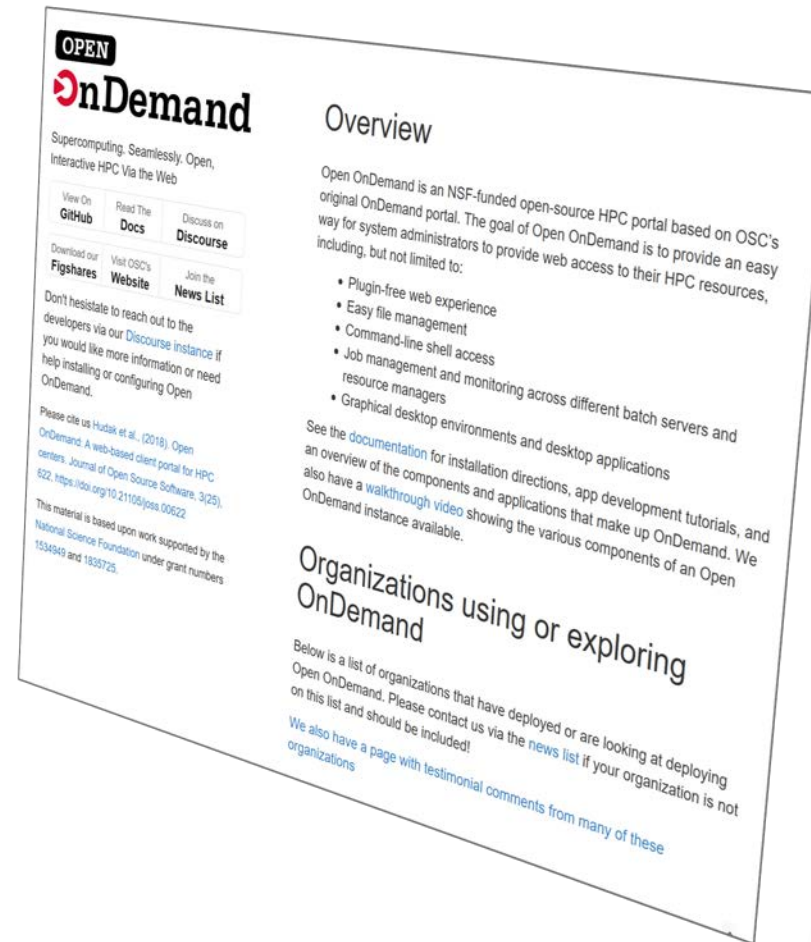


# OPENONDEMAND.ORG

Use our Discourse instance for help

Join our mailing list for updates

Our webinars are roughly quarterly

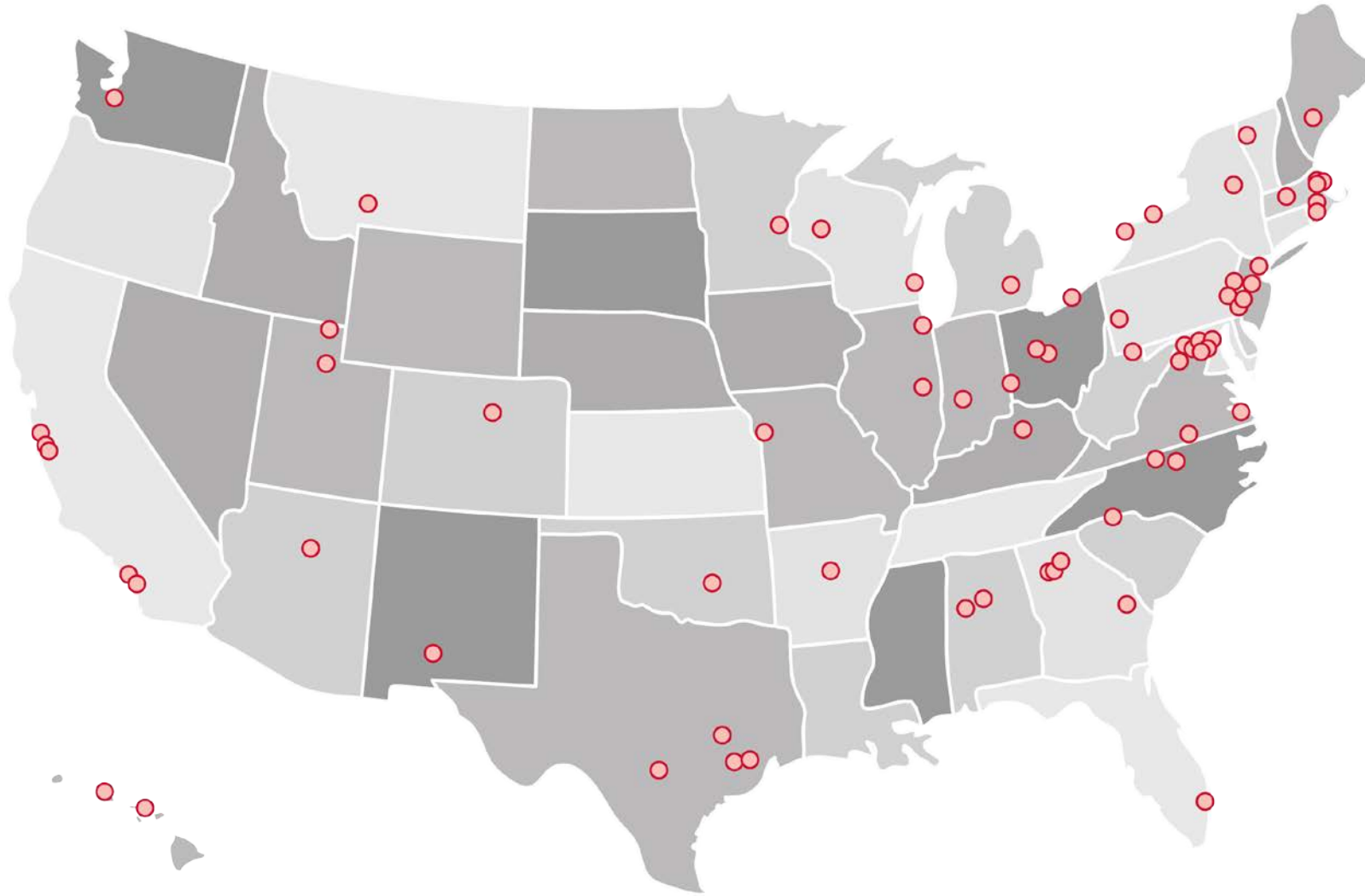


This work is supported by the National Science Foundation of the United States under the awards NSF SI2-SSE-1534949 and CSSI-Software-Frameworks-1835725.





## Approx Number of Institutions based on RPM logs



- 136 unique US locations
- 70 unique international locations







# Example Current Engagements and Deployments

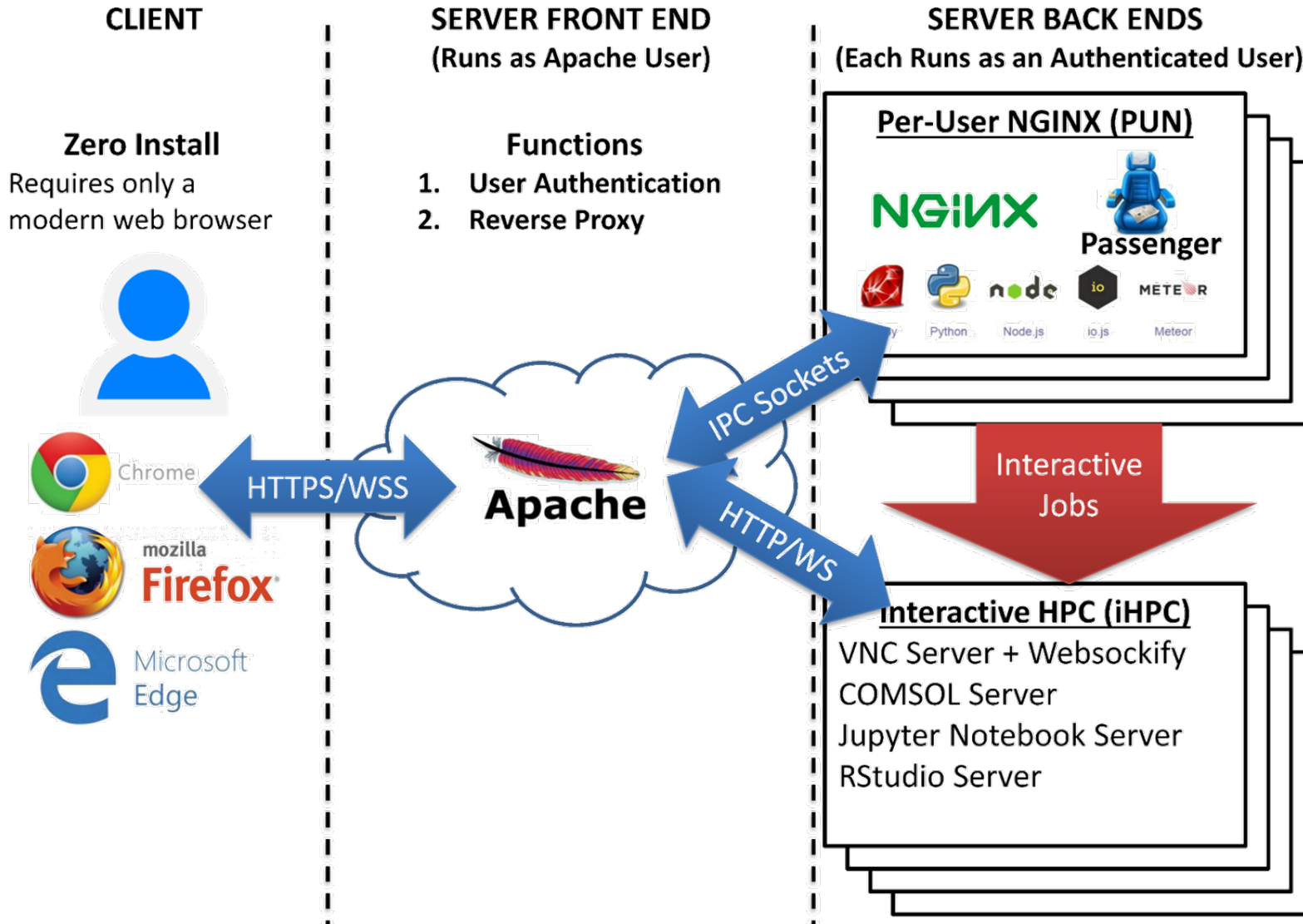
## In Process of Installing

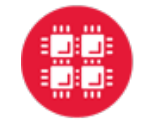


## Production Deployments









# Open OnDemand 2.0 Project Overview

Previous three year NSF SI2 award (#1534949) to develop OnDemand 1.x

Awarded follow on NSF CSSI award (#1835725) to develop OnDemand 2.x

Project runs from Jan 2019 to Dec 2023

Collaborators include SUNY Buffalo and Virginia Tech

## Four areas

**Visibility:** Enhancing resource utilization visibility by integrating the existing Open XDMoD platform

**Scalability:** support more types of computing resources and software

**Accessibility:** appeal to more scientists in more fields of science

**Engagement:** establish community of departmental, campus and national HPC users and administrators





## Check out the Project on GitHub

See all the projects at: <https://github.com/OSC/ondemand/projects>

Large features currently stated for release: <https://github.com/OSC/ondemand/projects/10>

Feel free to comment or react to tickets. Open feature requests or anything. We want to hear from you!



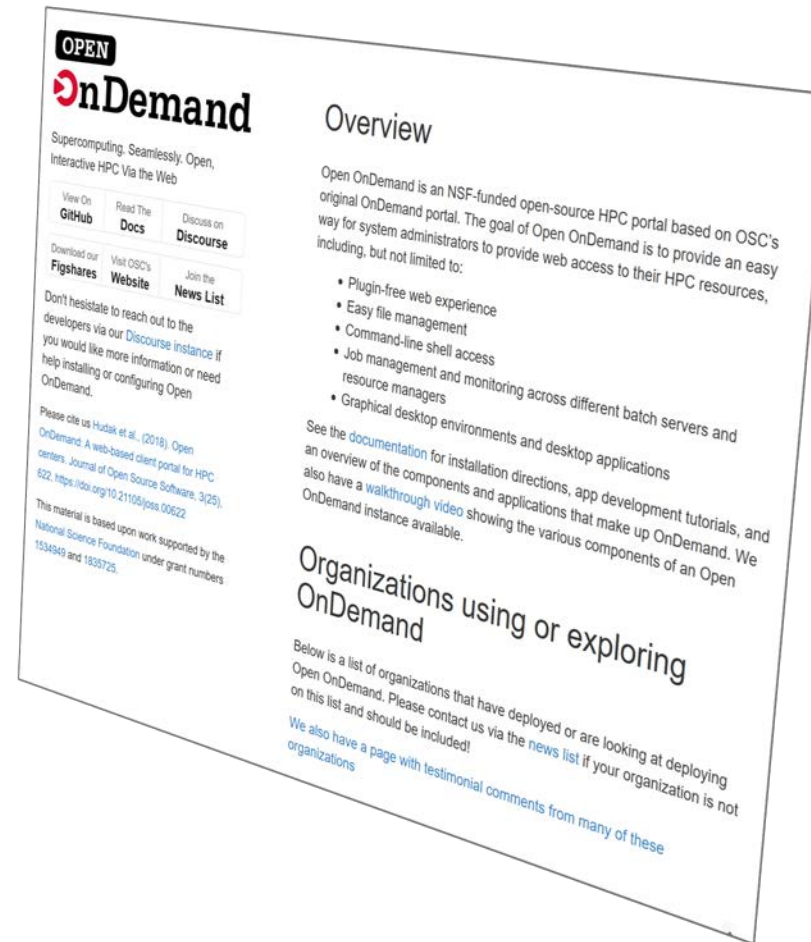


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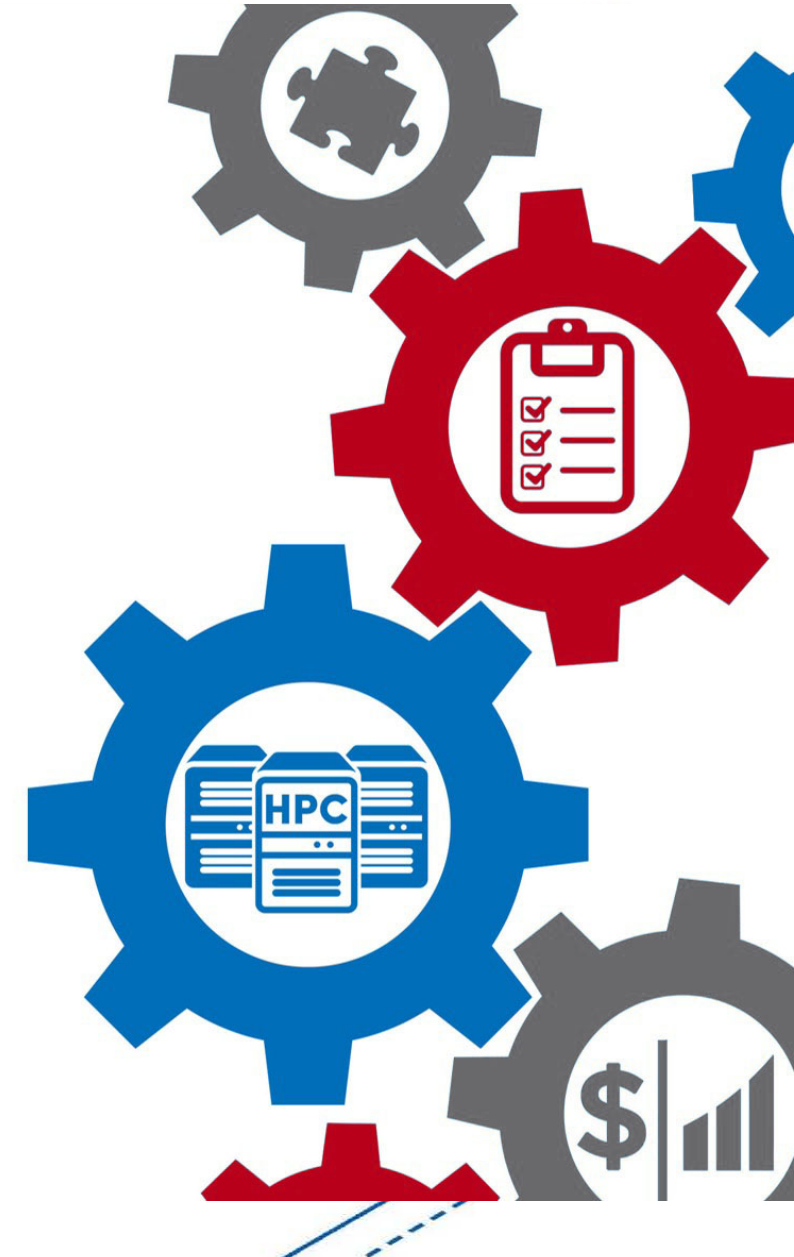
This work is supported by the National Science Foundation of the United States under the awards NSF SI2-SSE-1534949 and CSSI-Software-Frameworks-1835725.





# Usage Overview Demo

Alan Chalker - OSC

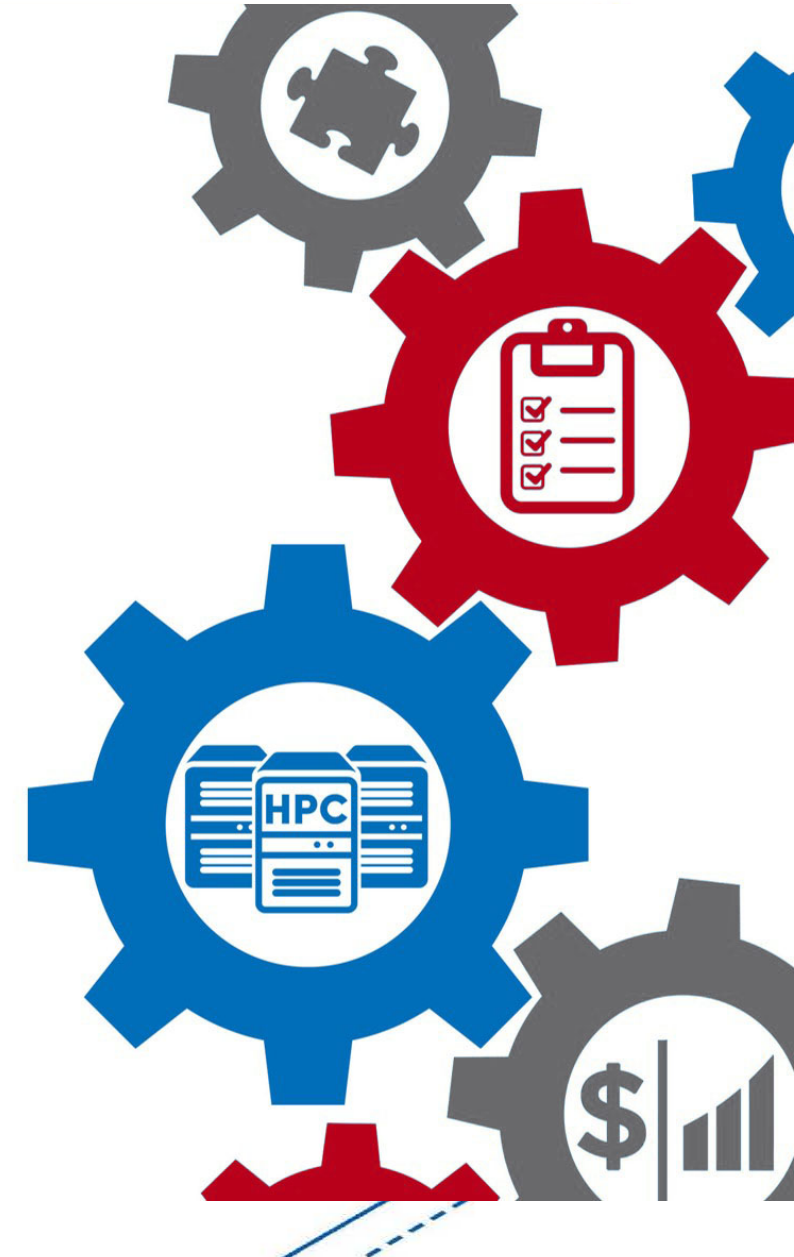






# Configuring software to be available in OnDemand

Jeff Ohrstrom - OSC





## Configuring software to be available in OnDemand

- New software is made available through OnDemand by adding new “apps”
- Users can develop and run apps in their home directory
- Admins can publish apps by copying them to the OnDemand web host’s local disk in `/var/www/ood/apps`





## Configuring software: Types of apps

- **Interactive App Plugins**
  - Consists of a job template and configuration files
  - Submits a batch job which launches VNC GUI app or web server on compute node and provides user link to connect
- **Passenger web apps written in Python, Ruby, or Node.js**
  - run as the user - they are acting behalf of the user
  - do not need to manage authentication or authorization
  - write any app specific data to user dirs (\$HOME, \$SCRATCH)





# Hands on Tutorial: Dashboard in Development Mode

## It Covers:

- Setting up the dashboard in development mode
- Changing the navigation bar color
- 2.0 Features:
  - Pinning Apps to the dashboard
  - Changing the layout of the dashboard
  - Adding custom widgets to the dashboard





# Dashboard Tutorial: Pinning Apps to the dashboard

- Pinning Apps and then grouping them

Open OnDemand Apps Files Jobs Clusters Interactive Apps

**OPEN**  
**OnDemand**  
OnDemand provides an integrated, single access point for all of your HPC resources.

Pinned Apps A featured subset of [all available apps](#)

- HPC Cluster Shell Access (System Installed App)
- Active Jobs (System Installed App)
- Home Directory (System Installed App)
- Desktop (System Installed App)
- Job Composer (System Installed App)
- Jupyter Notebook (System Installed App)

Open OnDemand Apps Files Jobs Clusters Interactive Apps

**OPEN**  
**OnDemand**  
OnDemand provides an integrated, single access point for all of your HPC resources.

Pinned Apps A featured subset of [all available apps](#)

**Clusters**

- HPC Cluster Shell Access (System Installed App)

**Files**

- Home Directory (System Installed App)







# Dashboard Tutorial: Changing the layout

- Change the layout so that Message of the Day is on the left

Before

Open OnDemand Apps Files Jobs Clusters Interactive Apps My Interactive Sessions Develop Help Logged in as hpcadmin Log Out

**OPEN OnDemand**  
OnDemand provides an integrated, single access point for all of your HPC resources.

Pinned Apps A featured subset of all available apps

**Clusters**

HPC Cluster Shell Access  
System Installed App

**Files**

Home Directory  
System Installed App

**Message of the Day**

**Tutorial links**

- Coldfront: <https://localhost:2443>
- OnDemand: <https://localhost:3443>
- XDMoD: <https://localhost:4443>
- Login to frontend: `ssh -p 6222 hpcadmin@localhost`
- GitHub Repo: <https://github.com/ubccr/hpc-toolset-tutorial>
- Accounts: <https://github.com/ubccr/hpc-toolset-tutorial/blob/master/docs/applications.md>
- OnDemand Tutorial: <https://github.com/ubccr/hpc-toolset-tutorial/blob/master/ondemand/README.md>

**Project links**

- Coldfront: <https://github.com/ubccr/coldfront>
- OnDemand: <https://openondemand.org>
- XDMoD: <https://open.xdmod.org>

**Notes**

Get the public environment for using Jupyter

After

Open OnDemand Apps Files Jobs Clusters Interactive Apps My Interactive Sessions Develop Help Logged in as hpcadmin Log Out

**OPEN OnDemand**  
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**Message of the Day**

**Tutorial links**

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- Accounts: <https://github.com/ubccr/hpc-toolset-tutorial/blob/master/docs/applications.md>
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**Notes**

Get the public environment for using Jupyter

Pinned Apps A featured subset of all available apps

**Clusters**

HPC Cluster Shell Access  
System Installed App

**Files**

Home Directory  
System Installed App



# Dashboard Tutorial: Adding a new widget

- Add a new custom widget

The screenshot shows the Open OnDemand dashboard interface. At the top is a dark green navigation bar with the following items: "Open OnDemand", "Apps", "Files", "Jobs", "Clusters", "Interactive Apps", "My Interactive Sessions", "Develop", "Help", "Logged in as hpcadmin", and "Log Out".

Below the navigation bar is the "OPEN OnDemand" logo and a sub-header: "OnDemand provides an integrated, single access point for all of your HPC resources." A light blue banner below this reads: "Thank you for attending the PEARC 2021 Open OnDemand Tutorial!"

The main content area is divided into two columns:

- Left Column:**
  - Message of the Day:** A section with a horizontal line below the title.
  - Tutorial links:** A list of links:
    - Coldfront: <https://localhost:2443>
    - OnDemand: <https://localhost:3443>
    - XDMoD: <https://localhost:4443>
    - Login to frontend: `ssh -p 6222 hpcadmin@localhost`
    - GitHub Repo: <https://github.com/ubccr/hpc-toolset-tutorial>
    - Accounts: <https://github.com/ubccr/hpc-toolset-tutorial/blob/master/docs/applications.md>
    - OnDemand Tutorial: <https://github.com/ubccr/hpc-toolset-tutorial/blob/master/ondemand/README.md>
  - Project links:**
    - Coldfront: <https://github.com/ubccr/coldfront>
- Right Column:**
  - Pinned Apps:** A section titled "A featured subset of all available apps".
  - Clusters:** A dark blue header for a section containing a card for "HPC Cluster Shell Access". The card shows a terminal icon, the text "HPC Cluster Shell Access", and "System Installed App".
  - Files:** A dark blue header for a section containing a card with a house icon.





# Hands on Tutorial: Create a Jupyter “Interactive App Plugin”

## It Covers:

- Getting the app to work.
- Checking logfiles to debugging failures.
- Changing the types of form items
  - From text input to select widgets
- Adding new form options
- Using Native scheduler options
- Explanations of files
- Promoting the app to production





## Jupyter Tutorial: Get the App working

- Jupyter example application doesn't work out of the box
  - Configure it to use this cluster
  - Configure it to use the correct Jupyter installation
- The card is shown when a successful Jupyter job is launched

**HPC Tutorial Jupyter (2)** 1 node | 1 core | Running

Host: `>_cpn01` Delete

Created at: 2020-07-21 19:27:37 UTC

Time Remaining: 59 minutes

Session ID: b71ea2ba-83ec-40ea-9011-7dd5b834b31f

---

[Connect to Jupyter](#)





## Jupyter Tutorial: Modify the Partition

- Change the partition element to be a select dropdown instead of a text field


**Partition**


  
**Compute**  
Debug




# Jupyter Tutorial: Deploy to production

- Deploy the app to production for other users

Interactive Apps
Desktops
 HPC Desktop

Tutorial Apps
Machine Learning
 HPC Tutorial Jupyter

Tutorial Apps [Sandbox]
Machine Learning
 HPC Tutorial Jupyter







## Jupyter Tutorial: Set the memory request for the job

- Use the script.native attributes to set the --mem SLURM argument

Memory (MB)

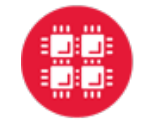


RSS Memory

Launch

\* The HPC Tutorial Jupyter session data for this session can be accessed under the [data root directory](#).





## Jupyter Tutorial: Limit the number of nodes

- Put an upper limit on the number of nodes allowed

### Number of nodes

17

Please select a value that is no more than the number of nodes available when the session starts.

\* The HPC Tutorial Jupyter session data for this session can be accessed under the [data root directory](#).





## Jupyter Tutorial: Add a checkbox to start JupyterLab

- Add a checkbox so users can boot JupyterLab or Jupyter Notebook

Use JupyterLab instead of Jupyter Notebook?

JupyterLab is the next generation of Jupyter, and is completely compatible with existing Jupyter Notebooks.

Launch

\* The HPC Tutorial Jupyter session data for this session can be accessed under the [data root directory](#).





## Jupyter Tutorial: Delete unused fields

- Delete unused fields to clean up the form

### Partition

Compute

### Number of hours

1

### Number of nodes

1

### Memory (MB)

600

RSS Memory

Use JupyterLab instead of Jupyter Notebook?

JupyterLab is the next generation of Jupyter, and is completely compatible with existing Jupyter Notebooks.

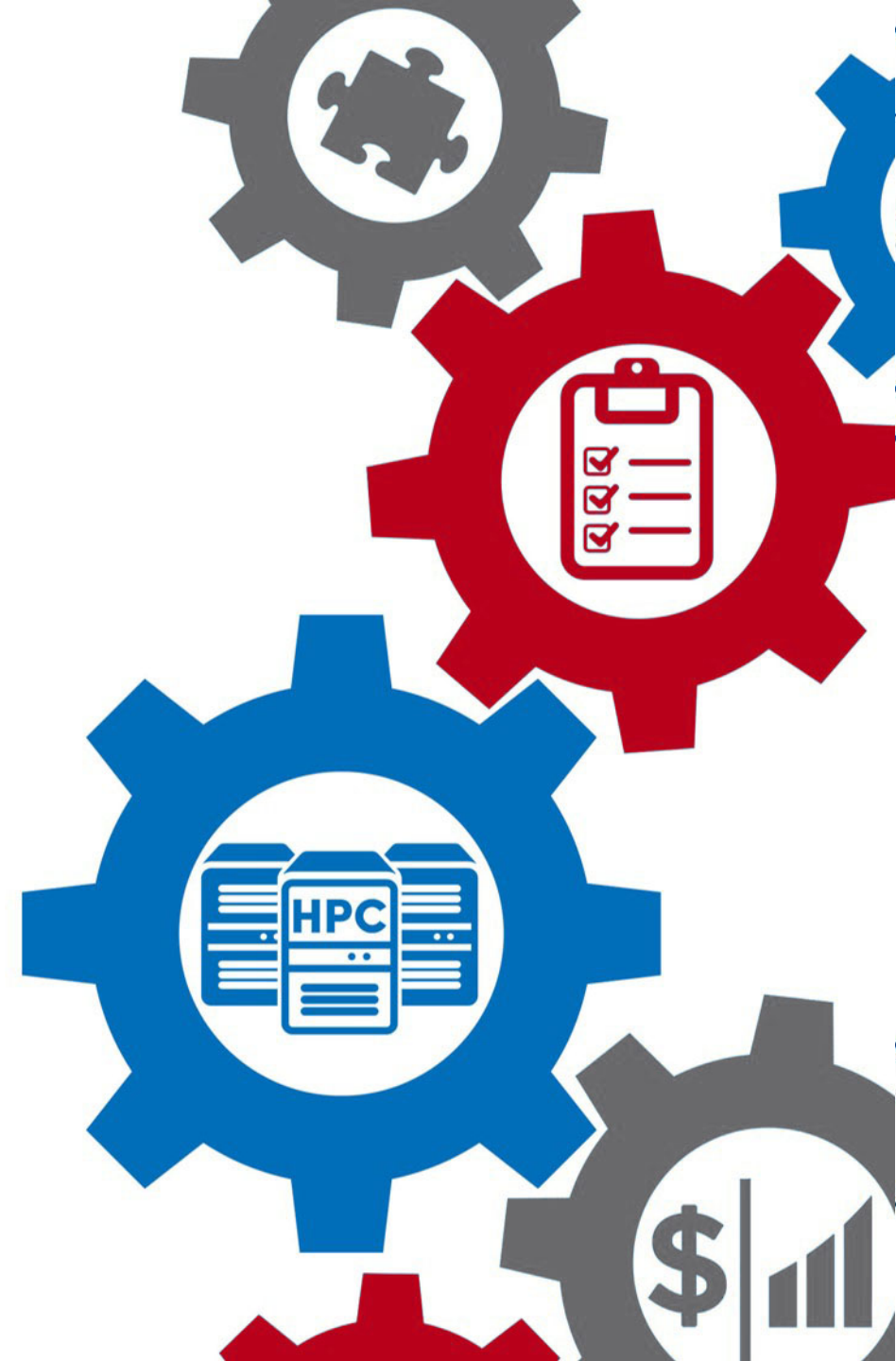
Launch

\* The HPC Tutorial Jupyter session data for this session can be accessed under the [data root directory](#).



# Break

OSC has a job opening on the Open OnDemand team! Full details here:  
[go.osu.edu/ood-job](https://go.osu.edu/ood-job)



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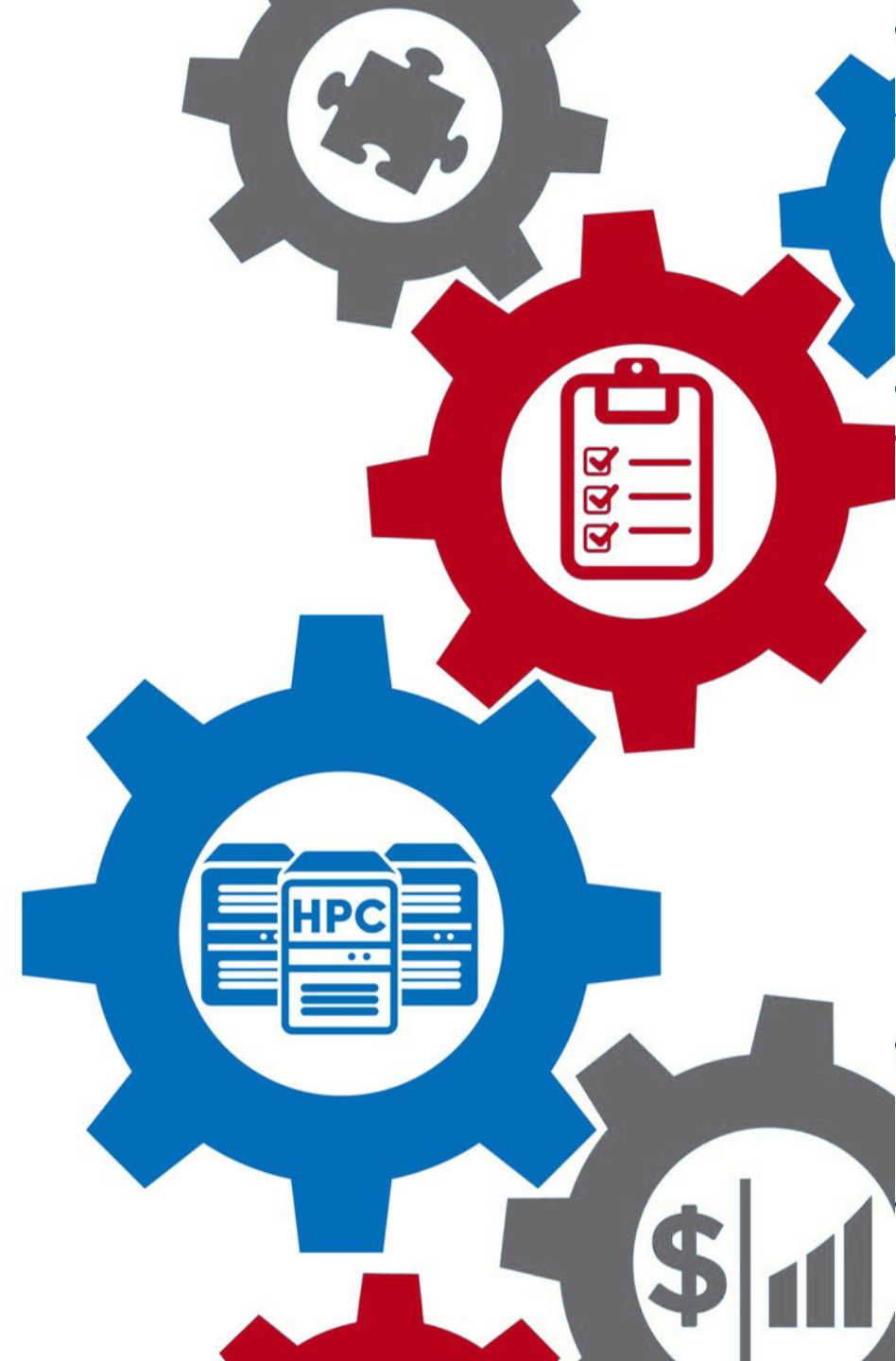
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# XDMoD and OnDemand Integration

Jeff Ohrstrom - OSC



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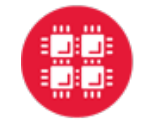


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## Overview of integration

- Presents job efficiency reports from XDMoD directly on the OnDemand dashboard
- Integration enabled by user being logged into both XDMoD and OnDemand
- Only works if authenticated using same OpenID Connect or SAML Identity Provider
- This should be available in OnDemand 1.8 and XDMoD 9





## Enabling the XDMoD reports on OnDemand dashboard

1. Configure OnDemand with XDMoD host URL in PUN  
`/etc/ood/config/nginx_stage.yml`
2. Configure OnDemand with XDMoD resource id in each cluster config  
`/etc/ood/config/clusters.d/hpc.yml`
3. Add OnDemand host as domain to XDMoD portal settings for CORS  
`/etc/xdmod/portal_settings.ini`
4. Configure identity provider to include OnDemand host in HTTP Content-Security-Policy for frame-ancestors since OnDemand uses iFrames to trigger SSO with XDMoD when a user logs in





## Benefits of integrating XDMoD and OnDemand

1. Encourage users, even those new to HPC to access to historical job information through XDMoD
2. Provide faster access to relevant job information XDMoD from OnDemand
3. Ensure that users with poorly performing jobs are encouraged to fix them by presenting reports with red graphs every time they log into OnDemand





## Future plans

1. Completed Jobs App
2. Server side integration to address Single Sign On problems by moving communication to the server
3. Provide OnDemand usage metrics through XDMoD

The screenshot shows a web browser window with the URL `ondemand-test.osc.edu/pun/dev/completedjobs`. The page title is "OSC OnDemand / Completed Jobs". Below the title, there is a "Completed Jobs" section with a "Show 50 entries" dropdown and a "Filter:" input field. The main content is a table with columns: ID, Job Name, Start Time, Time Used, Cluster, and CPU Graph. The table contains six rows of job data, each with a small CPU graph icon in the CPU Graph column.

ID	Job Name	Start Time	Time Used	Cluster	CPU Graph
931595 - XDMoD	STDIN	Nov 4, 2019 2:43:37 pm	00:00:01	Pitzer	
8366776 - XDMoD	ondemand/sys/myjobs/basic_blast	Nov 4, 2019 12:29:00 pm	00:30:31	Owens	
8366777 - XDMoD	ondemand/sys/myjobs/basic_lammps_parallel	Nov 4, 2019 12:30:28 pm	00:02:07	Owens	
8357609 - XDMoD	ondemand/sys/dashboard/sys/bc_osc_rstudio_server	Nov 1, 2019 5:01:16 pm	01:00:07	Owens	
8357574 - XDMoD	ondemand/sys/dashboard/dev/matlab	Nov 1, 2019 4:40:09 pm	01:00:25	Owens	
8357572 - XDMoD	ondemand/sys/dashboard/dev/matlab	Nov 1, 2019 4:38:38 pm	00:01:01	Owens	

Find more ways to help users optimize their jobs!







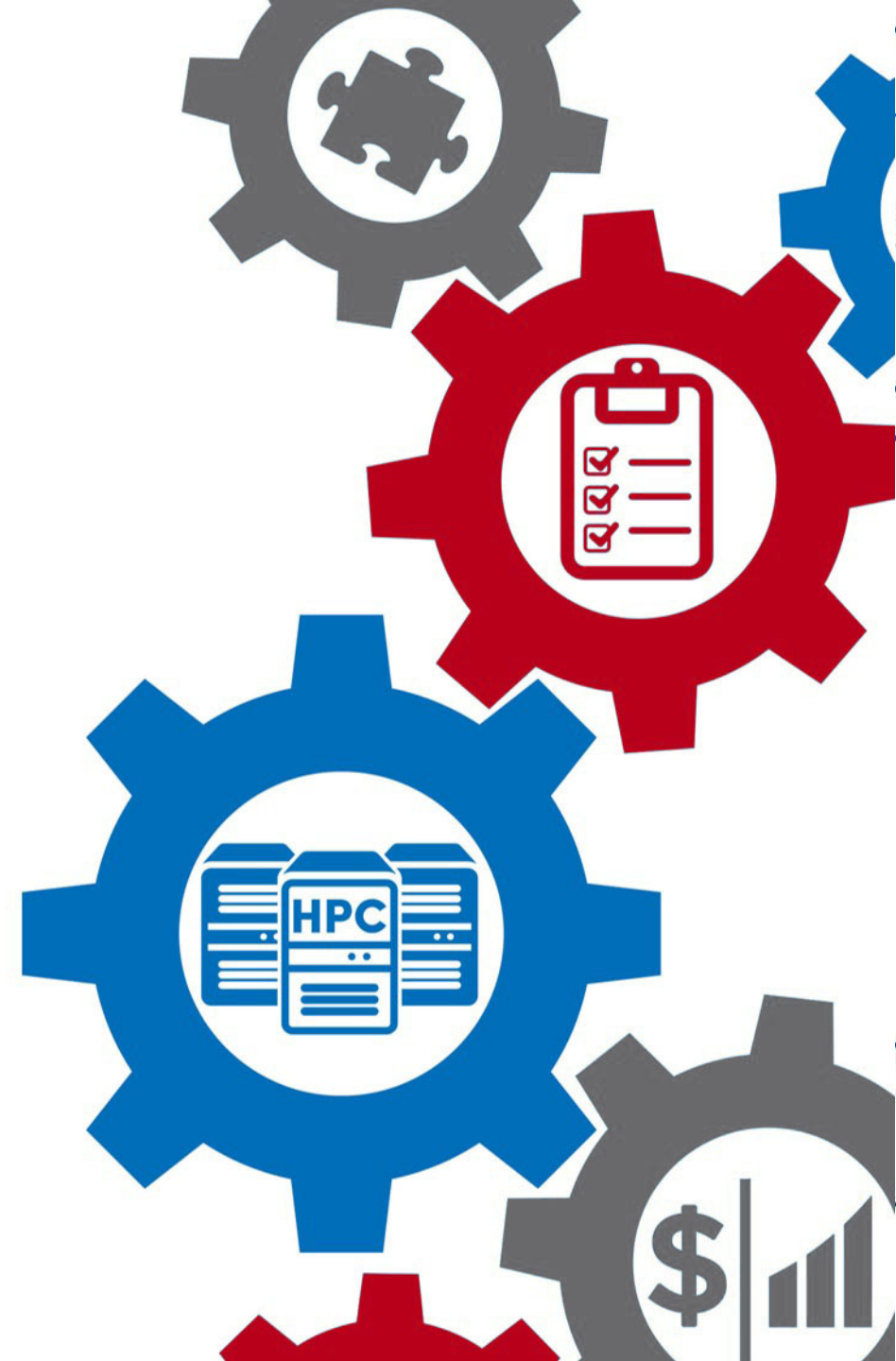
## Funding and other acknowledgements:

- OnDemand is supported by the National Science Foundation – award numbers [NSF#1534949](#) and [NSF#1935725](#)
- Open XDMoD is supported by the National Science Foundation – award numbers [ACI 1025159](#) and [ACI 1445806](#)
- We gratefully acknowledge the partnership with [Virginia Tech](#) on our current joint NSF project



# Thank you...

OSC, VT, and UB staff and students for helping with the tutorial today!



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## How to reach us:

Center for Computational Research – <https://buffalo.edu/ccr>

Open XDMoD - <https://open.xdmod.org/>

ColdFront - <https://github.com/ubccr/coldfront>

Ohio Supercomputer Center - <https://www.osc.edu/>

OnDemand - <https://openondemand.org/>

Virginia Tech – Advanced Research Computing - <https://arc.vt.edu/>





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**Join the staff & developers of  
each product immediately  
following this tutorial  
in the breakout rooms**

**Feel free to move between  
the rooms at any time**



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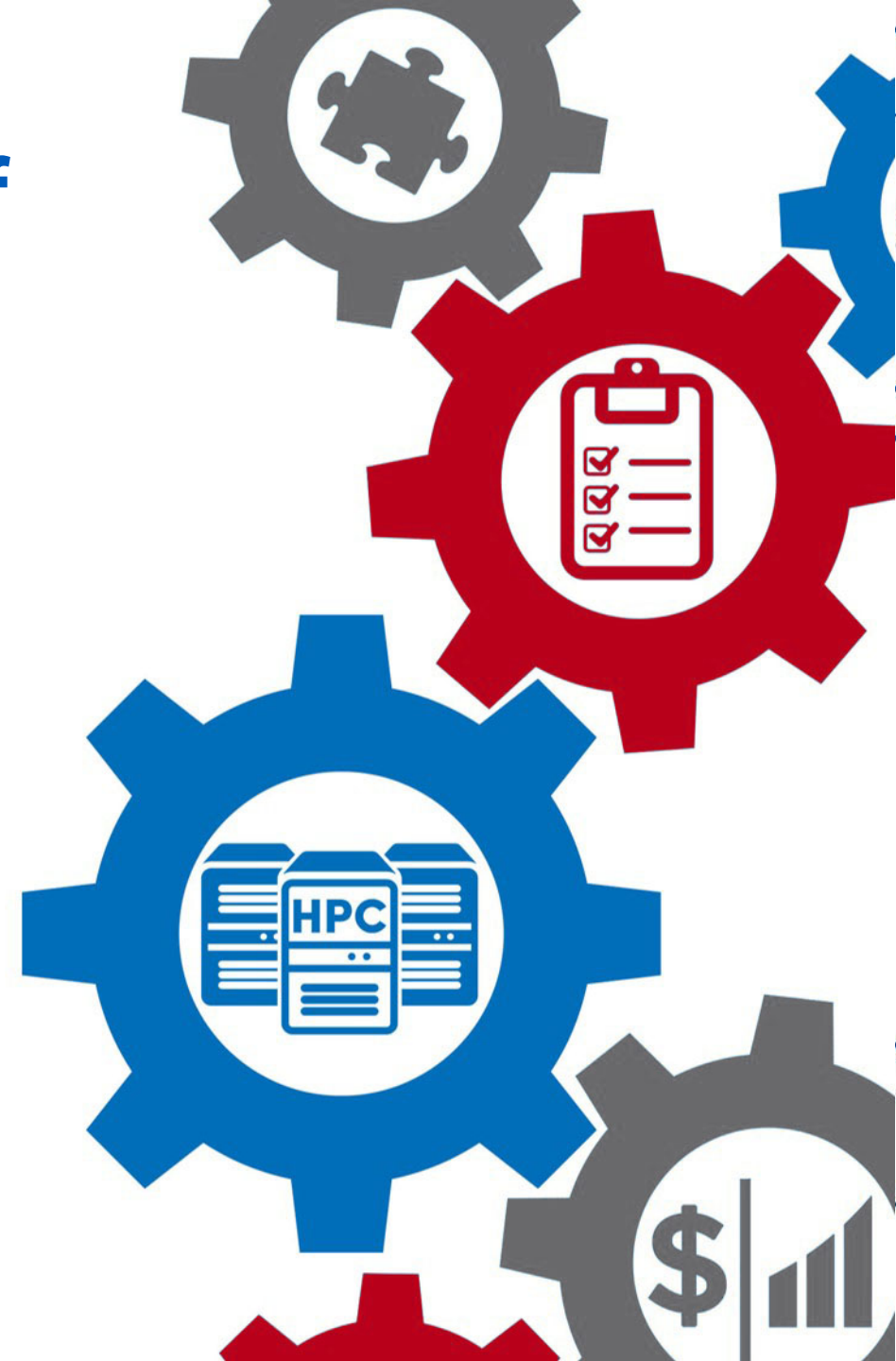


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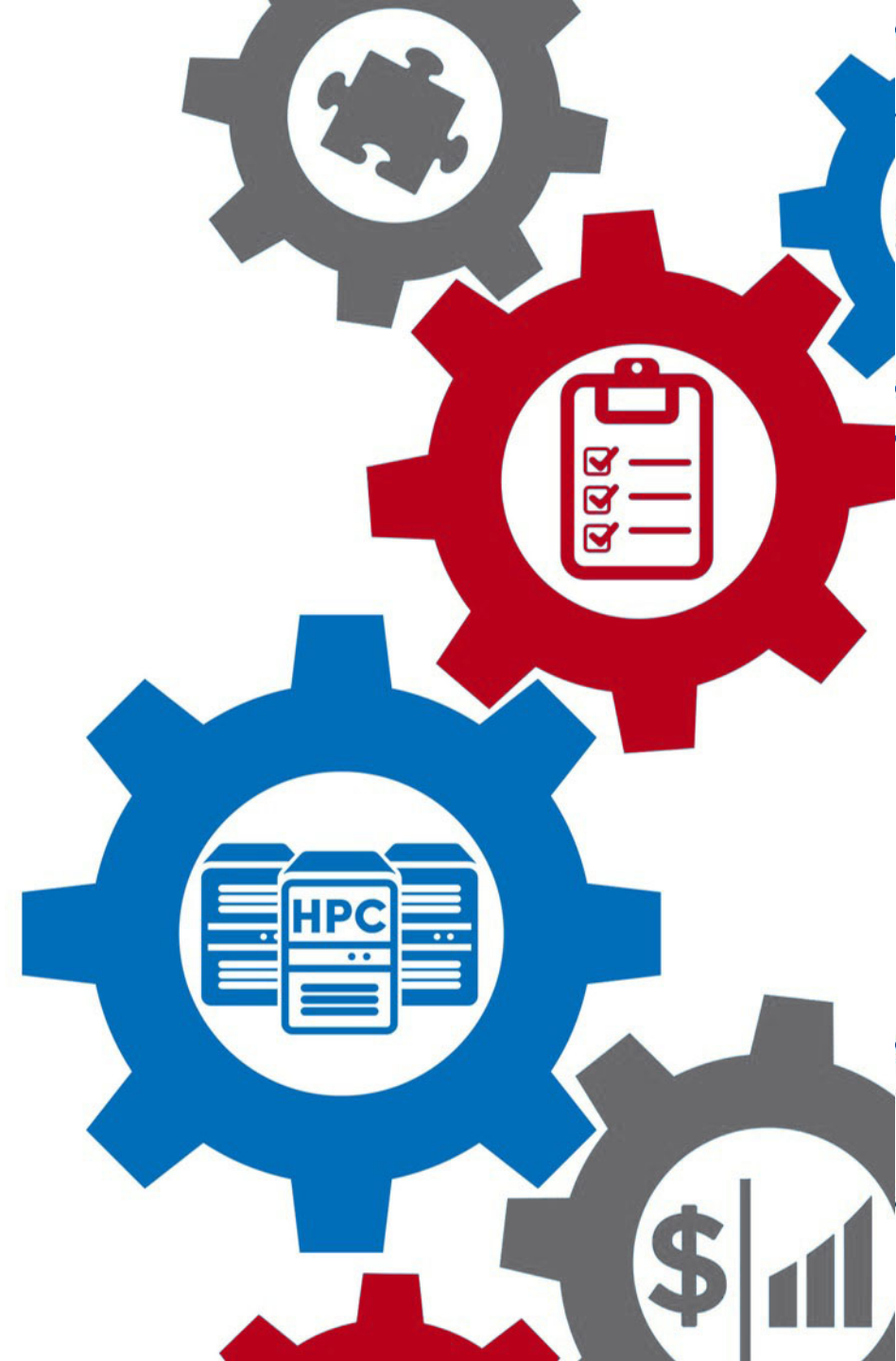
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# Thank you for attending!

Please fill out the post-tutorial survey

We value your opinions!



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