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

Tutorial presented at PEARC 2023 by staff from:

Ohio Supercomputer Center University at Buffalo Center for Computational Research

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

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



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In-Person Tutorial Staff:

Alan Chalker, OSC Jeff Ohrstrom, OSC Ryan Rathsam, UB Travis Ravert, OSC Dori Sajdak, UB Andrew Stoltman, UB

Contributing Tutorial & Product Dev Staff:

Andrew Bruno, UB Alan Chalker, OSC Andrew Collins, OSC Robert DeLeon, UB Trey Dockendorf, OSC David Hudak, OSC Matt Jones, UB Joseph White, UB



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Agenda

- Tutorial Goals
- Brief intro on all three products
- Tutorial technology & getting help
- Part 1: ColdFront
- 9:45-10:15am: Break
- 10:15-10:45am: ColdFront (con't)
- 10:45-11:30am: Part 2: Open OnDemand
- 11:30am-1pm: Lunch
- 1-2:15pm: OnDemand (con't)
- 2:15-3pm: Part 3: Open XDMoD
- 3-3:30pm: Break
- 3:30-4:20pm: XDMoD (con't)
- 4:20-4:30pm: Wrap up & Q&A



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Tutorial Goals:

- First presented at PEARC 2020 (virtually)
- Provide participants with an introduction to each product
- Demonstrate the features that allow the products to work together
- 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



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ColdFront – Managing Access

- Used as the source of record in an 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 (Slurm), 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)



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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



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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





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Tutorial Container Architecture



Requirements: <u>https://github.com/ubccr/hpc-toolset-</u> 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 20+GB 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.

WARNING!!! DO NOT run these containers on production systems. This project is for educational purposes only. The container images we publish for the tutorial are configured with hard coded, insecure passwords and should be run locally in development for testing and learning only.





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Tutorial Walk Through

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

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

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





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Getting Help

- Join the Slack organization for the tutorial <u>https://tinyurl.com/hpctoolset</u>
- What to do if you're having a technical problem:
 Slack us or raise your hand & we'll do our best to help out

Remember: all of this is available after the tutorial so you can just sit back and watch





Tutorial presented at PEARC 2023 by:

Dori Sajdak Senior Systems Administrator, UB CCR



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What is ColdFront?



HPC resource allocation management system

Integrates with 3rd party apps for automation & access control

Intuitive Portal for users, system admins, & center staff Self-service project management for faculty, ROI data collection for you

Source of truth for your center

Centralized info, better security, customized for your workflow and policies

Open source, written in python, extensible with Django apps, *active community* that contributes to the project



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Access Control





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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 their 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





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ColdFront – 3 Major Parts

Resources

Anything you want to control access to and/or monitor usage of

Allocations

Determine what resource an account has access to & for how long

Projects

Contain project info, users, allocations, & reportable data (publications, grants, etc)





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Resources

- Resources might include:
 - clusters, cluster partitions, storage platforms, cloud, servers, scientific instruments, databases, software licenses
- Resources have attributes
 - Some might restrict access & tie into plugins for automation:
 - Cluster config options Slurm plugin
 - System access or filesystem access restricted by UNIX group FreeIPA plugin
 - Some might be informational:
 - End user license agreements
 - Warranty expiration dates
- Metadata allow for fine grain control
 - Is the resource private or public?
 - Available only to certain users/groups?
 - Is the resource a child resource of a larger (parent) resource?
- The attributes set on resources are inherited by allocations
- These attributes are customizable



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Allocations

- Determines what resource a user account has access to & for how long
- Allocation attributes may set limits, restrict access, and/or tie into the ColdFront plugins. Examples include:
 - Slurm account name
 - Total number of CPU/core hours allowed
 - UNIX group
 - Storage quota
- Allocation Change requests allow requesting & updating attribute values
- Allocation attributes are customizable
- Allocation metadata includes start & end, creation & last modified dates, status, description, associated resource(s) & justification
- Users emailed when end date is imminent configurable time spans
- If allocation isn't renewed & expires access to the resource is removed for everyone on the allocation



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Projects

- Project = users, allocations for resources, reportable data (publications, grants), project attributes, description, field of science
- PIs (group manager) 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



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System administrator views of allocation requests

Allocation Requests

#	Date Requested/ Last Modified	Project Title	PI	Resource	Project Review Status	Status	Allocation Actions
1	Apr. 01, 2021	my project	cgray cgray (cgray)	hpc cluster (Cluster)		New	Activate Deny

Allocation Requests & Change Requests Can be Viewed by System Administrators

Allocation Change Requests

For each allocation change request below, there is the option to activate the allocation request and to view the allocation change's detail page. If a change request is only for an extension to the allocation, they can be approved on this page. However if the change request includes changes to the allocation's attributes, the request must be reviewed and acted upon in its detail page.

#	Requested	Project Title	PI	Resource	Extension	Actions
24	Jan. 13, 2022	Testing Storage 1	Dori Sajdak (djm29)	ProjectStorage (Storage)	60 days	Approve Details
27	Jan. 14, 2022	Testing Storage 1	Dori Sajdak (djm29)	BudgetStorage (Storage)	60 days	Approve Details





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Annual Project Reviews

You cannot request a new allocation because you have to review your project first.

You need to review this project. Review Project

Test Project

👶 Manage Project

Reviewing Project: Test Project

CCR requires faculty to review their project information annually in order to renew their group's accounts. The information provided by researchers is compiled and used to help make the case to the University for continued investment in CCR. Up-to-date and accurate information is crucial to our success. Questions? Contact us

Please update the following information:

1.	Verify your project description is accurate
2.	Add Publications
3. 🗹	Add Grants
4. 🗹	Verify the user accounts in your group and remove any that should no longer have
	and the second

Grants Last Updated:	Sep. 11, 2018
Publications Last Updated:	Sep. 11, 2018
Users in project:	Dori Sajdak

access to CCR resources

Reason for not updating project information*

If you have no new information to provide, you are required to provide a statement explaining this in this box. Thank you!

Completed Annual Project Reviews Can be Viewed by Center Director and System Admins

Pending Project Reviews

	Date Review		Grants Last	Publications Last	Reason for not Updating	
Project Title	Submitted	PI	Updated	Updated	Project	Project Review Actions
My Test Project	May. 13, 2021	Dori Sajdak (djm29)	May. 13, 2021	May. 13, 2021		Mark Complete Email



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🏆 User Grants Summary



Grants Total: \$375,027,785 Grants Total PI Only: \$179,766,586 Grants Total CoPI Only: \$152,122,982 Grants Total Senior Personnel Only: \$43,138,217

Center Directors can better demonstrate the center's impact

- Collect publication & grant info
- Research output other work product
- Enforce annual updates of info project description, field of science
- Other ROI information?





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Extensible plug-in architecture allows for integration of nearly anything! OpenID (0) workload manager OPEN Vendor APIs **On Demand**

METRICS ON DEMAND



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https://www.osc.edu/ https://openondemand.org/ **University at Buffalo**

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https://buffalo.edu/ccr https://open.xdmod.org/ https://coldfront.io

NOW: Break: 30 minutes

Coming Up! Part 1: ColdFront (con't) Part 2: Open OnDemand

Important Info:

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XDMoD BOF: Wed, 7/26 1:30-2:30PM - E146

Open OnDemand Booth - During Exhibition Hall hours



OPEN ON Demand **Overview &** Walk-through

Alan Chalker **Travis Ravert Jeff Ohrstrom**

Ohio Supercomputer Center











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Why Run Open OnDemand?

Zero installation

Run Open OnDemand entirely in your browser. No client software installation required.

Easy to use

Start computing immediately. A simple interface makes Open OnDemand easy to learn and use.

Compatible with any device

Launch on any device with a browser—even a mobile phone or tablet.

Access your organization's supercomputers through the web to compute from anywhere, on any device.



openondemand.org/run



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Why Install Open OnDemand?

Low barrier to entry

Empower users of all skill levels by offering an alternative to command-line interface.

Free and open source

Install Open OnDemand for free, and gather knowledge from our large open-source community.

Configurable and flexible

Create and deploy your own applications to meet your users' unique needs.

Administer remote web access to your supercomputers to transform the way users work and learn.



openondemand.org/install





Example Deployments



openondemand.org/orgs



Don't see an organization?

The more the merrier! Let us know any that belong on the list





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Community Events

Tips and tricks calls

Hosted by the larger Open OnDemand community, tips and tricks webinars share best practices for setting up and using Open OnDemand. They take place on the first Thursday of every month at 1 p.m. ET.



Open office hours

Hosted by our development team, Zoom open office hours are the perfect opportunity to ask questions or make a suggestion. They are held on the second Tuesday of every month from 11:15 a.m. to 12:45 p.m. ET.



PEARC Booth / BoF

Visit the Open OnDemand table (#10)

Attend our User Group BoF, Tues (July 25), 1:00 – 2:30 p.m. Room F150

openondemand.org/events



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Need Support?

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Discuss on Discourse

The Get Help thread on our Discourse forum features user and admin questions and answers. Browse recent questions or leave one of your own.



Documentation

Our documentation outlines installation steps, app development guidelines, release notes, and more. Search for a specific topic or browse for general info.

openondemand.org/support



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Demo Topics

Dashboard landing page

File management

Batch jobs / job composer

Viewing active jobs

Interactive applications

Dashboard profiles



openondemand.org/demo



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

https://buffalo.edu/ccr https://open.xdmod.org/ https://coldfront.io

NOW: Lunch – 90 minutes

Important Info:

<u>Coming Up – starting at 1:30pm</u> Part 2: Open OnDemand (con't) Part 3: Open XDMoD

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XDMoD Overview

Ryan Rathsam, Andrew Stoltman Center for Computational Research University at Buffalo







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XDMoD: Metrics on Demand

Comprehensive framework for CI system management

Compute Jobs, Storage, Cloud, and Networking

Understand and optimize resource utilization and performance

- Provide instantaneous and historical information on utilization
- Measure Quality of Service of CI systems and applications
- Measure and improve job and system level performance
- Inform computing system upgrades and procurements

ACCESS XDMoD tool

• Analytics Framework for XSEDE/ACCESS

Open XDMoD*: Open Source version for CI centers

- Used to measure and optimize performance of CI centers
- 400+ academic, governmental, & commercial installations worldwide
- <u>https://open.xdmod.org/</u>





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Benefits for Stakeholders

PI and End User

Account management, resource selection, application tuning, improved throughput

Systems Administrator

System diagnostic and performance optimization, application tuning

Center Support Staff

- Diagnose Job Failure / Performance Issues
- Identify users who may need additional help

CI Center Director

- Comprehensive resource management and planning tool
- Return on Investment Metrics





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Why Improving CI Performance Matters

CI systems are oversubscribed

- Improving application or system performance improves overall job throughput
- Frees up otherwise wasted CPU cycles for useful work

Small improvements in performance can have high impact

- Every 1% increase in system performance on the resources provided through XSEDE translates into the ability to allocate an additional 101 M CPU hours annually
- Corresponds to a savings of \$5M*





* Assuming a rate of \$0.05 per CPU hour



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XDMoD Portal

- Web-based
 - Point and click drill down capability
- Display metrics
 - Utilization, performance, scientific impact
- Role based access
 - User
 - Principal Investigator
 - Center Staff ۲
 - Center Director

Custom Report Builder



Metric

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NOW: Break: 30 minutes

Coming Up! Part 3: Open XDMoD (con't) Wrap up and Q&A

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Thank you for attending!

Please fill out the post-tutorial survey

We value your opinions!



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Funding and other acknowledgements:

- OnDemand is supported by the National Science Foundation award numbers <u>NSF#1534949</u> and <u>NSF#1935725</u>
- Open XDMoD is supported by the National Science Foundation award numbers <u>ACI</u> <u>1025159</u> and <u>ACI 1445806</u> and <u>OAC 2137603</u>
- We gratefully acknowledge the partnership with Virginia Tech on our current NSF project





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Staff are available after the tutorial concludes for specific questions. Please continue to engage with us and the user communities on Slack!





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QUESTIONS?

How to reach us:

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

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

ColdFront - https://coldfront.io

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

OnDemand - https://openondemand.org/

