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

**Tutorial presented at ISC 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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#### University at Buffalo

Center for Computational Research





Center for Computational Research

### **In-Person Tutorial Staff:**

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Agenda

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- Tutorial Goals
- Brief intro on all three products
- Tutorial technology & getting help
- Part 1: ColdFront
- Part 2: Open OnDemand
- Break: 11-11:30am
- Part 3: Open XDMoD
- Post Workshop utilize the slack channel, attend the OnDemand User Group "Birds of a Feather" session Wednesday at 3pm, visit the OnDemand booth





# **Tutorial Goals:**

- 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





### **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)





## **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





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## **Tutorial Container Architecture**

**HPC Toolset Containers** 



Requirements: https://github.com/ubccr/hpc-toolsettutorial/edit/master/docs/requirements.md

#### **Clone the Github Repo:**

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

cd hpc-toolset-tutorial

./hpcts start

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\* The first time you do this, you'll be download ~20GB 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 https://tinyurl.com/hpctoolset
- 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 ٠ back and watch

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Channels . coldfront # # general # isc23 ondemand # a tutorial\_staff xdmod #



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**Tutorial presented at ISC 2023 by:** 

Dori Sajdak Senior Systems Administrator, UB CCR



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# What is ColdFront?



## HPC resource allocation management system

Integrates with 3<sup>rd</sup> 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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## Why We Developed ColdFront:

- System Administrators wanted: •
  - More automation, less manual error
  - One location for access management of all resources

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- Allow Pls 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

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- 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 ٠
- 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





## 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





## 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





### System administrator views of allocation requests

### **Allocation Requests**

#	Date Requested/ Last Modified	Project Title	Ы	Resource	Project Review Status	Status	Allocation Ac	ctions
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

\lambda 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

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4. Z Verify the user accounts in your group and remove any that should no longer have access to CCR resources

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

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

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



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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?



#### Total Publications: 1979



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# Extensible plug-in architecture allows for integration of nearly anything! OpenID **FreeIPA** Open Source Identity Management Solution

Vendor APIs



workload manager





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## Integrations

Plug-ins (Django Apps)

- <u>OnDemand</u>
- **XDMoD**
- Slurm ۲
- Mokey/Hydra OpenID Connect (Identity Management)
- FreeIPA (LDAP/AD) ۲
- Other plug-in examples
- Other 3<sup>rd</sup> party APIs should be added as a new plug-in (Django app)

Community Plugins: **OpenStack** Keycloak User Search Starfish

Courtesy of: New England Research Cloud Harvard FAS Research Computing Group

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# **ColdFront Technology**

• Requirements: Python 3.6+

Uses the Django web framework

- Recommend 'pip' for easy install
- What you'll need for production:
  - Gunicorn
  - MariaDB/MySQL, PostgreSQL, or SQLite
  - Django Q (qcluster)
  - redis
  - nginx (recommended)
  - SSL (strongly recommended)

### https://coldfront.readthedocs.io/en/latest/deploy/

### Hardware Requirements?

- Very lightweight, minimal disk space, 1 CPU, little RAM
- CCR production instance is a VM w/2 VCPUs & 8GB of RAM (of which almost nothing is in use!)





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# **Tutorial Steps:**

Pre-seed the database: This creates different user roles and access, creates a new cluster resource, and sets up a ٠ project for our PI user. These steps are detailed out in the repo instructions should you want to go through them yourself later

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- As PI user: add a user, conduct project review, request allocation change & request allocation ٠ renewal
- As the center director user: check out Project Review process, view other menu options
- As sys admin user, review allocations & allocation change requests and sync with Slurm
- As the PI user, run a batch job, then click on OnDemand logo to move to next part of tutorial ٠



### **Contact Info:**

Dori Sajdak - djm29@buffalo.edu

https://coldfront.io

More about UB CCR: https://buffalo.edu/ccr https://twitter.com/ubccr



HPC



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### **Brian Guilfoos**

HPC Client Services Manager

Ohio Supercomputer Center



Chio Supercomputer Center An OH·TECH Consortium Member

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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





# 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**

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CHALMERS CHAPMAN CHALMERS CHAPMAN CORVIDINERSITY CORVIDINE	do
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Kentucky LEHIGH	
UNIVERSITY OF A Microsoft Azure OF WISCHSIN	
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openondemand.org/orgs



# Don't see an organization?

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





# **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.



### ISC23 Booth / BoF

Visit the Open OnDemand booth (#E524)

Attend our User Group BoF, Weds (May 24) 3:10 – 4:10 p.m.



openondemand.org/events





# **Need Support?**

$\square$	

### **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





# **Demo Topics**

Dashboard landing page

File management

Batch jobs / job composer

Viewing active jobs

Interactive applications

Dashboard profiles



openondemand.org/demo

# **XDMoD Overview**

Ryan Rathsam Center for Computational Research University at Buffalo



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# Ohio Supercomputer Center An OH·TECH Consortium Member Center for Computational Research Metrics

# **Overview Outline**

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- Introduction
- Overview of Open XDMoD
  - XDMoD Portal
  - Measuring Quality of Service
  - Measuring job level performance
  - Integration with Open OnDemand

# Open XDMoD Demo





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# Metric

# Who Am I?

- Scientific Programmer
- Been a part of the XDMoD Team for 8 years

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 Security Advocate and Application **Security Specialist** 









**University at Buffalo** 

# **XDMoD: Metrics on Demand**

### Comprehensive framework for CI system management

HPC 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







# **Benefits for Stakeholders**

### PI and End User

• Account management, resource selection, application tuning, improved throughput

### Systems Administrator

System diagnostic and performance optimization, application tuning

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### Computational Scientist

• Tool to facilitate work with end-users to improve job performance and throughput

### CI Center Director

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

### External Reviewer

 Tool for data driven review for verification of best practices and project goals

### Senior Leadership

- Measure the effectiveness of supported programs
- Inform deployment of future systems to fulfill unmet need







### CI systems are oversubscribed

- Improving application or system performance improves overall job throughput
- Free's 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

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Corresponds to a savings of \$5M\*







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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
- Center Director

### Custom Report Builder



XDMOD Hello, Tom Furlani (logout) 🖽 Dashboard 🌽 My Profile 🕕 About 🔜 Roadmap 📝 Contact Us 🗸 🕐 Help Metric Explorer Allocations App Kernels Report Generator Compliance Sci Impact Job Viewer About Summary Usage - Start: 2016-06-13 🔄 End: 2018-06-13 🔄 🧳 Refresh | 🌆 Export | 🚔 Print | 🗋 Available For Repor 🖫 Load Chart + | 🔚 New Chart + 📳 Save As 😝 Save + 🎽 Undo (🎽 Redo | 🔚 Delete | 🎇 Add Data + 💉 🗡 Duick Filters + 🧒 Add Filter + 🌱 Filters + Wumber of jobs Number of Jobs and Total CPU Hours 7M 700M 6M Chart Options 600M Aggregate Timeseries 5M Add Data: 500M 3 Add Data Maccounts 😽 Add Filter Allocations Legend 4M 3M 3M 📸 Jobs Font Size 400M Log Scale Chart Requests Swap the X and Y axis Resource Allocations SUPREMM Single Y axis 300M Hide Tooltin Show Chart Filters in Subtitle Show in Summary tab 200M 2M 1M 100M Jul 2016 ep 2016 ov 2016 Jul 2017 ep 2017 ov 2017 XSEDE [Number of Jobs Ended] 2016-06-01 to 2018-06-13 Src: YDCDR Powered by YDMoD/Highchar 1 of 1 🕨 🕅 🗔 Show Remainder (Disable Pagi Page Description

Metric

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## **Easily Obtain Utilization Metrics**

### **CPU hours consumed by campus units**



CPU Hours Consumed by Decanal Unit Resource = ub-hpc



SCHOOL OF ENGINEERING AND APPLIED SCIENCES COLLEGE OF ARTS AND SCIENCES CONTERNAL NON-UB SCHOOL OF PUBLIC HEALTH AND HEALTH PROFESSIONS CENTER FOR COMPUTATIONAL RESEARCH CONTERS SCHOOL OF PHARMACY AND PHARMACEUTICAL SCIENCES COMPUTATIONAL SCHOOL OF MEDICINE AND BIOMEDICAL SCIENCES ROSWELL PARK INSTITUTE



METRICS ON DEMAND

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## **Drill Down for Greater Detail**

### **CPU** hours and jobs by Engineering Department



CPU Hours and Jobs by Dept in Engineering

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2013-01-01 to 2013-12-31 Src: HPcDB. Powered by XDMoD/Highcharts

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METRICS ON DEMAND

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# **QoS: Application Kernels**

### Computationally lightweight

• Run continuously and 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





**Measuring Job Level Performance** 

- Detailed job-level performance data
- Run on every cluster node and collects hardware counter data
  - CPU usage, Memory usage, I/O usage

### Identify poorly performing jobs (users) and applications





"Traffic Lights"

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Job employs 32 cores but only 1 core is active at a time with control swapping between the 32 cores Minor change to the submission script resulted in an improvement of a factor of 30



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## **Uses: Diagnosing Failed Jobs**





Metrics

- Job starts and memory usage rapidly increases on all nodes
- One of the compute nodes reaches the memory limit and fails
- FLOPS and L1D loads crash
- The job failed but still consumes all resources





# **Efficiency Tab**

METRICS ON DEMAND

### Facilitates user support

- Identify inefficient usage patterns and correct them
- Current efficiency metrics: CPU Usage, GPU Usage, Memory Usage, Homogeneity, Wall Time Accuracy, Short Jobs

#### What is this analytic?

The chart below shows the percentage of time that the GPUs were busy compared to overall usage. Each point on the plot shows the GPU jobs for a particular user.

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#### Why is this analytic important?

Making sure jobs use the right number of GPUs helps ensure that the compute resources are used efficiently.

#### How do I improve future jobs?

Try to ensure that the number of GPUs requested matches the number required. If a code is not using all GPUs adjust the configuration settings of the software to make use of all the requested GPUs or consider reguesting fewer GPUs in future jobs. If you have jobs with 0% GPU usage, double check that the code is compiled correctly to make use of the GPUs and is not defaulting to CPU-only calculations.

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## **XDMoD Data Analytics Framework**

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- Provide analytic framework for direct access to rich depository of performance and utilization data in XDMoD data warehouse
- No reliance on XDMoD web portal
- GUI Built on Jupyter notebooks
- Python and R interfaces for automated workflows and expert users



Metric





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Can access job viewer in

# **Open XDMoD - OnDemand Integration**

### Provide XDMoD information directly to OnDemand users



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# **OnDemand – Open XDMoD Integration**

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- View OnDemand usage in XDMoD
  - Who is using OnDemand?
  - What are they running?
  - Where are they running from? ۲







Number of Sessions

Metri



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# Demo

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Metrics



# **ACCESS MMS Team**

### University at Buffalo – Center for Computational Research

• Matt Jones, Bob DeLeon, Joe White, Nikolay Simakov, Ryan Rathsam, Gregary Dean, Conner Saeli, Andrew Stoltman, Aaron Weeden, Josh Furlani

**University at Buffalo** 

- Roswell Park
  - Tom Furlani (PI)
- TACC
  - Stephen Harrell, Matt Cawood (performance monitoring), Jennifer Schopf (Netsage)
- Tufts
  - Abani Patra (performance monitoring)
- Case Western
  - Vipin Chaudhary (application anomaly detection)
- SDSC
  - Shava Smallen (CloudBank)
- Support:
  - NSF Awards: 2137603, 1445806, 1025159









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Thank You!

## Questions?





# Danke! Thank you for attending!

Please fill out the post-tutorial survey

We value your opinions!



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- OnDemand is supported by the National Science Foundation award numbers ulletNSF#1534949 and NSF#1935725
- Open XDMoD is supported by the National Science Foundation award numbers ACI 1025159 and ACI 1445806 and OAC 2137603

**University at Buffalo** 

We gratefully acknowledge the partnership with <u>Virginia Tech</u> on our current NSF project ٠





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## Other places you'll find us at ISC 2023:

Open OnDemand User Group Meeting (BOF): Wed, 5/25 3:10-4:10pm

**University at Buffalo** 

**Booth #E524** - During Exhibition Hall hours

Staff are available after the tutorial concludes for specific questions. Please also join us on Slack!

https://tinyurl.com/hpctoolset





# Ohio Supercomputer Center I Center for Computational Research

## How to reach us:

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

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

ColdFront – <u>https://coldfront.io</u>

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

OnDemand - https://openondemand.org/

