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University at Buffalo
Center for Computational Research

VIRGINIA TECH

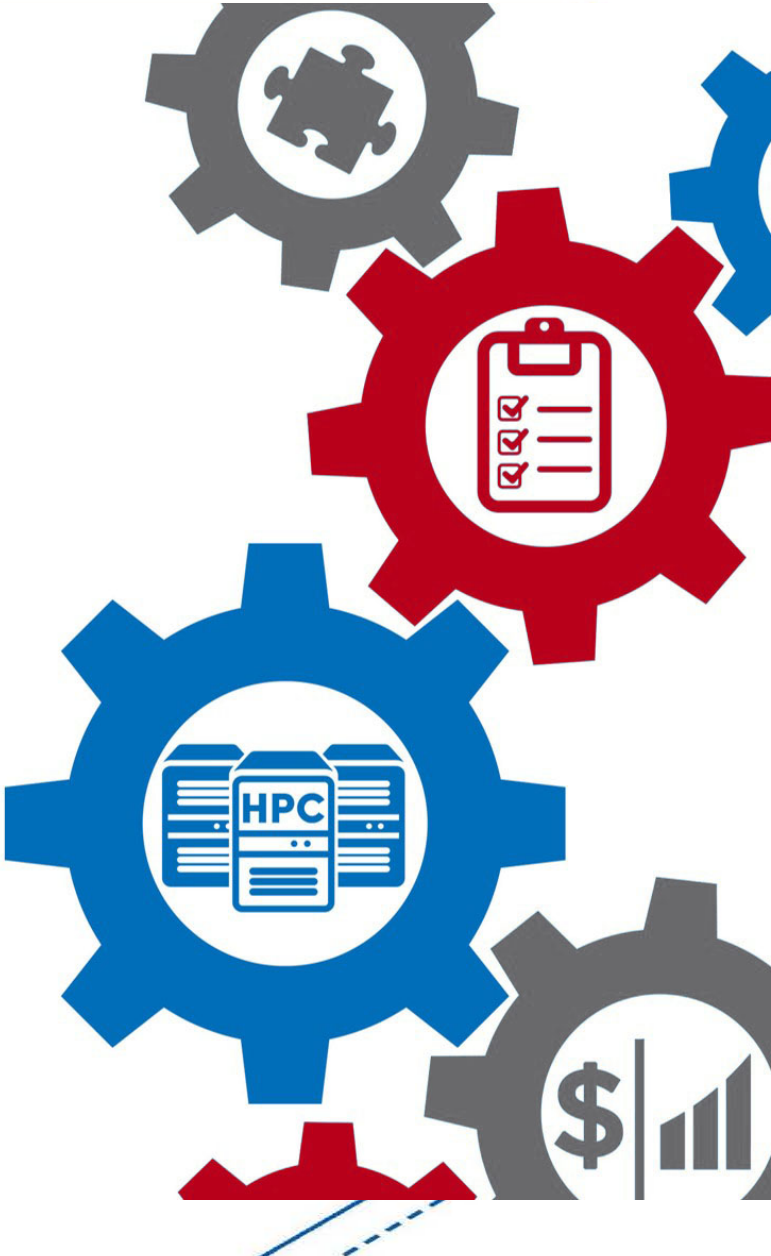
Open OnDemand, Open XDMoD, and ColdFront: An HPC center management toolset

WELCOME!

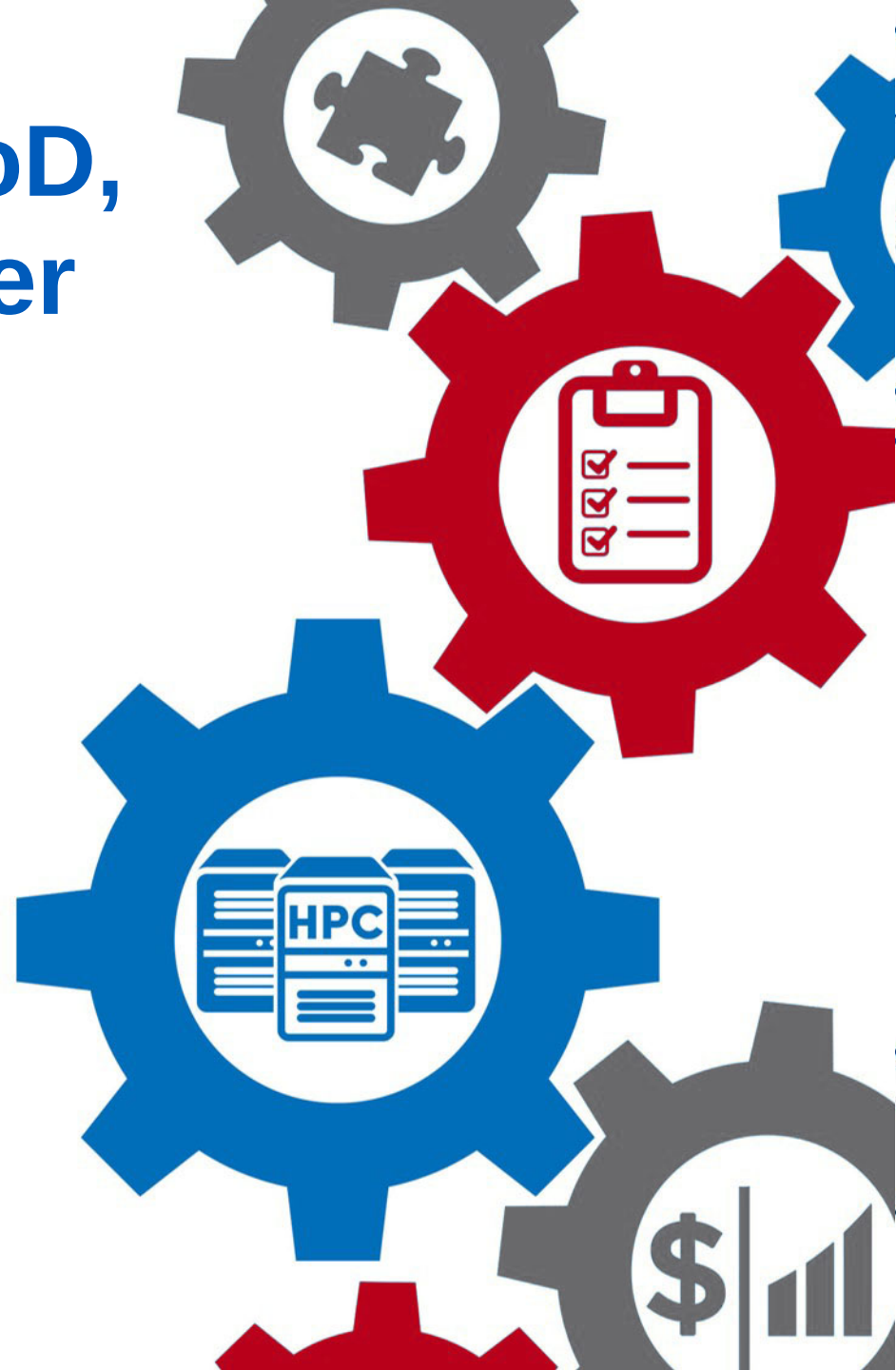
IF YOU HAVE NOT ALREADY DONE SO,
PLEASE FOLLOW SETUP INSTRUCTIONS!

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

Join the Slack organization for the tutorial
https://tinyurl.com/pearc-slack



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



Tutorial presented at PEARC22 by staff from:

Ohio Supercomputer Center

UB Center for Computational Research

Virginia Tech Advanced Research Computing

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Tutorial Staff:

Andrew Bruno, UB
Gerald Byrket, OSC
Alan Chalker, OSC
Andrew Collins, OSC
Robert DeLeon, UB
Trey Dockendorf, OSC
David Hudak, OSC
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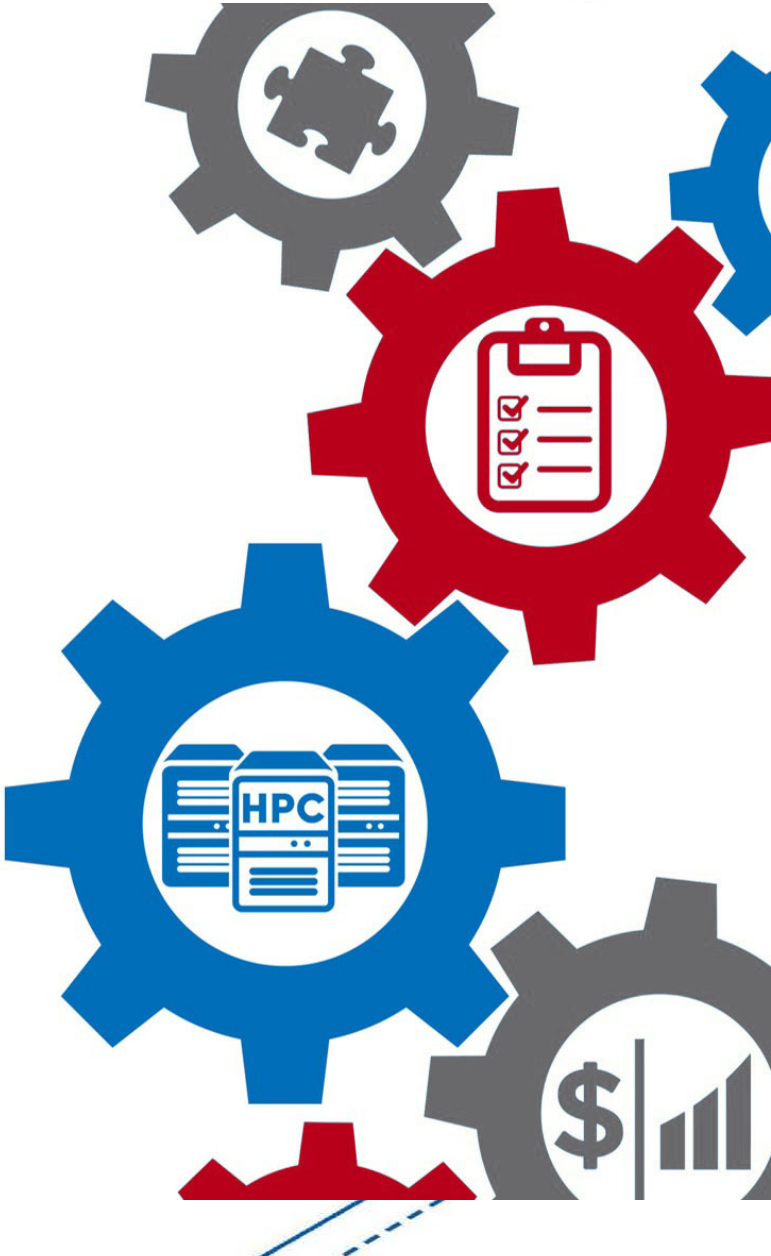
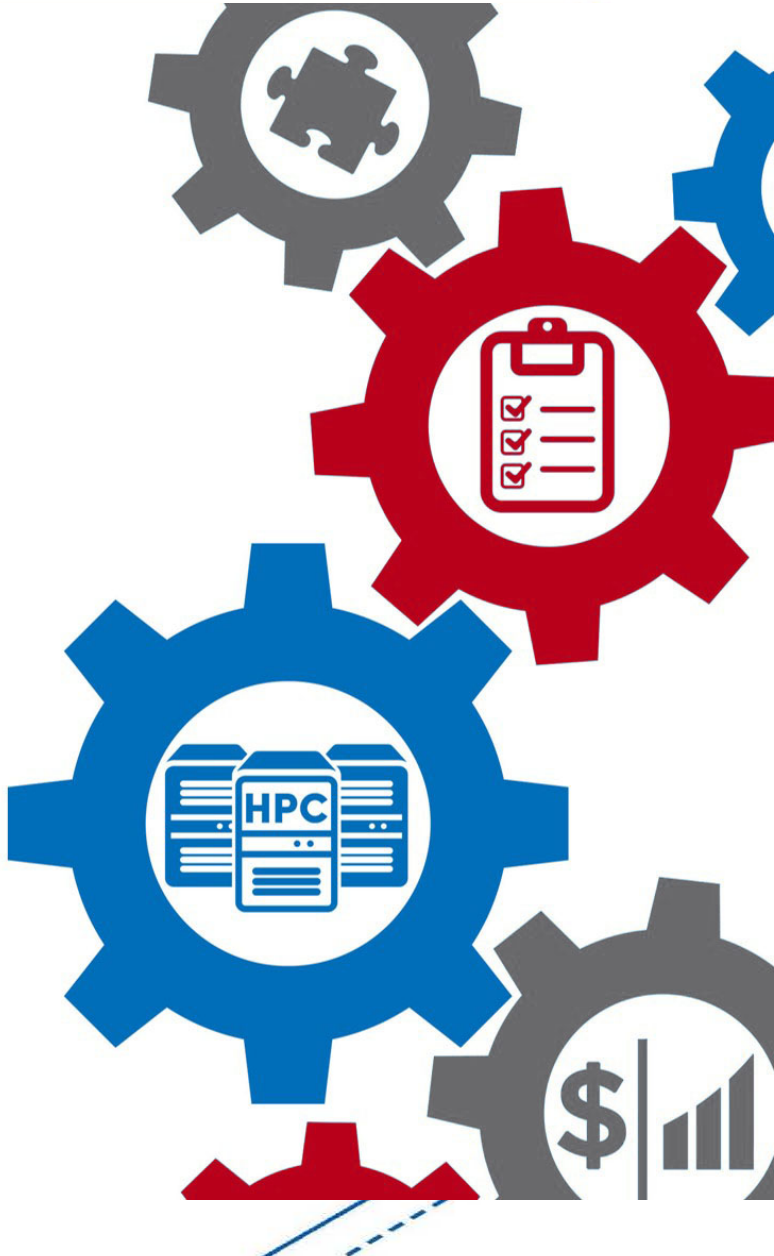
Travis Ravert, OSC
Dori Sajdak, UB
Bob Settlage, VT
Joseph White, UB



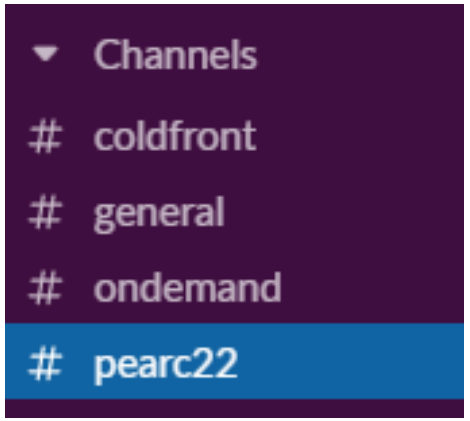
Agenda

- Getting Started & Tutorial Goals
- Brief intro on all three products
- Tutorial technology
- Part 1: ColdFront
- Break: 10-10:30am
- Part 2: Open XDMoD
- Lunch Break – 12-1:30pm
- Part 3: Open OnDemand
- Break: 3-3:30pm
- Part 4: Open OnDemand interactive app configuration
- Part 5: Dynamic Batch Connect Fields
- Post Workshop – breakout sessions & slack channel



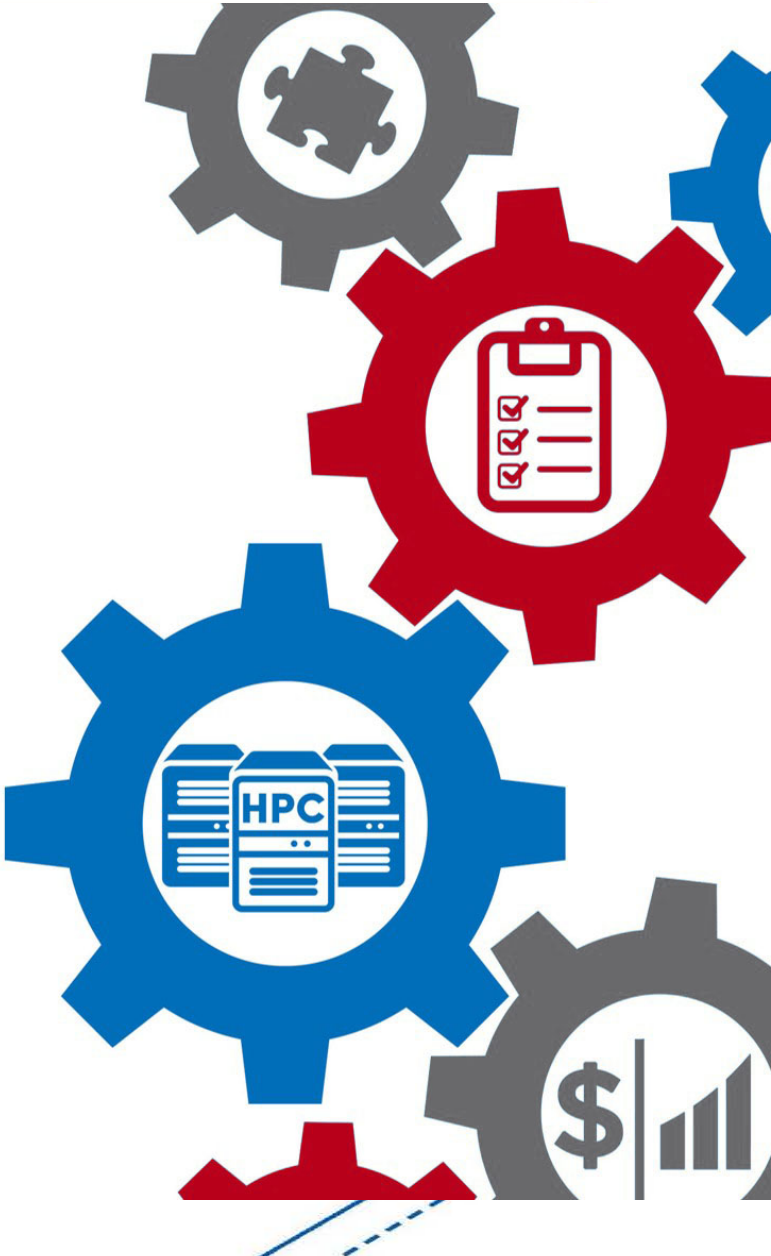
Getting Started

- Join the Slack organization for the tutorial
  https://tinyurl.com/pearc-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 – Slack us or raise your hand & we'll do our best to help out



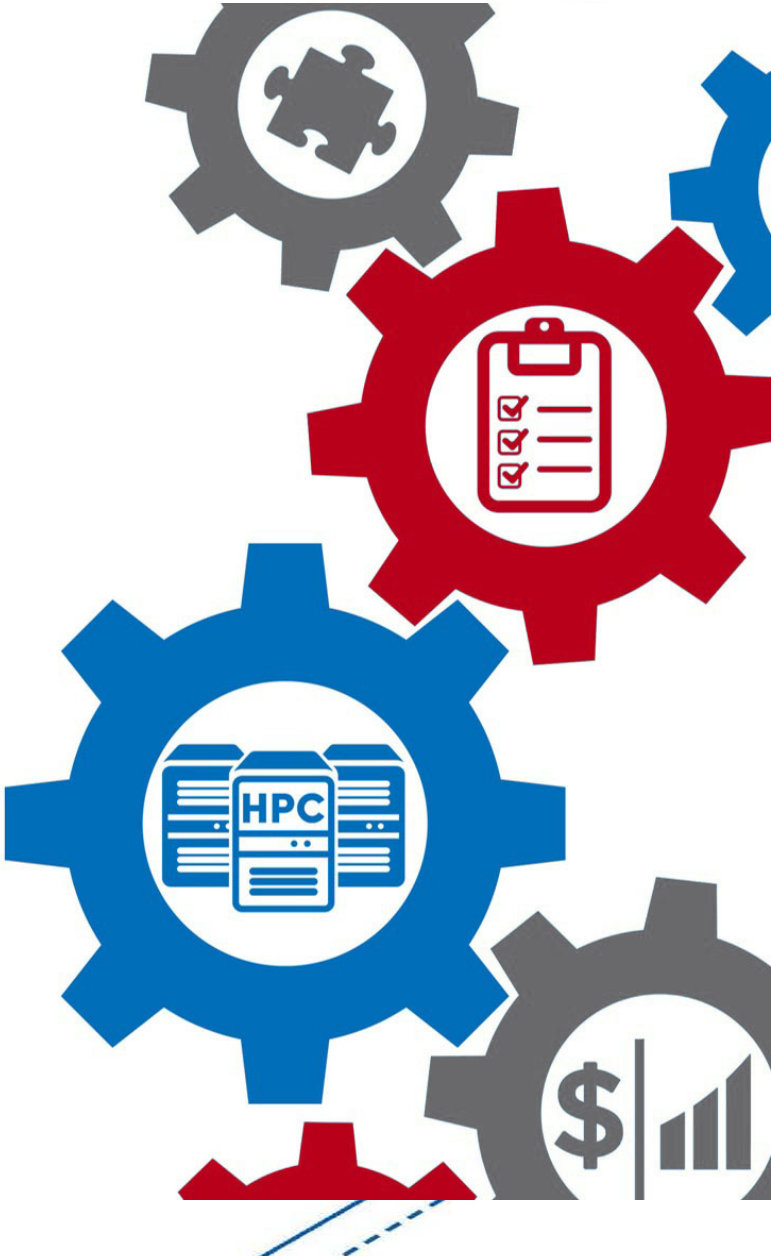
Tutorial Goals:

- Provide participants with an overview of each product & how they are installed/configured
- 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)

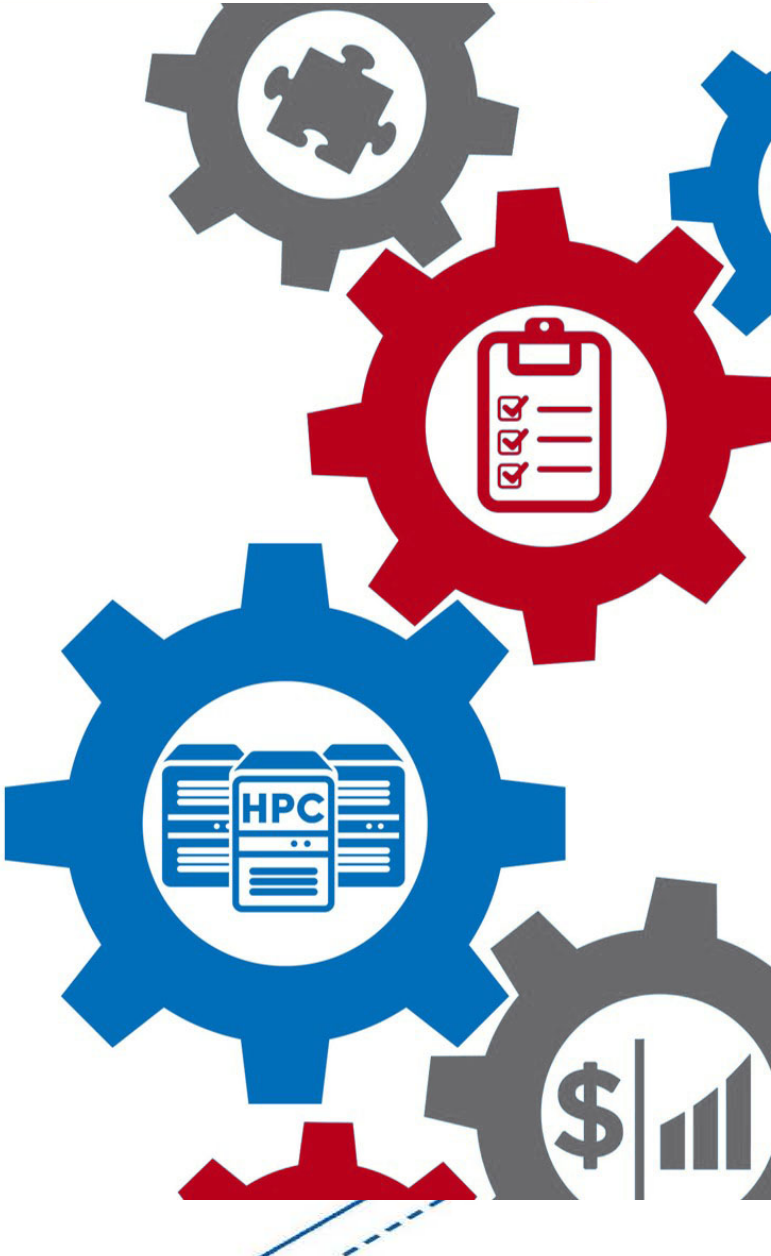


Open OnDemand – Easy Access

- Web-based portal for accessing HPC services that removes the complexities of HPC system environments from the end-user

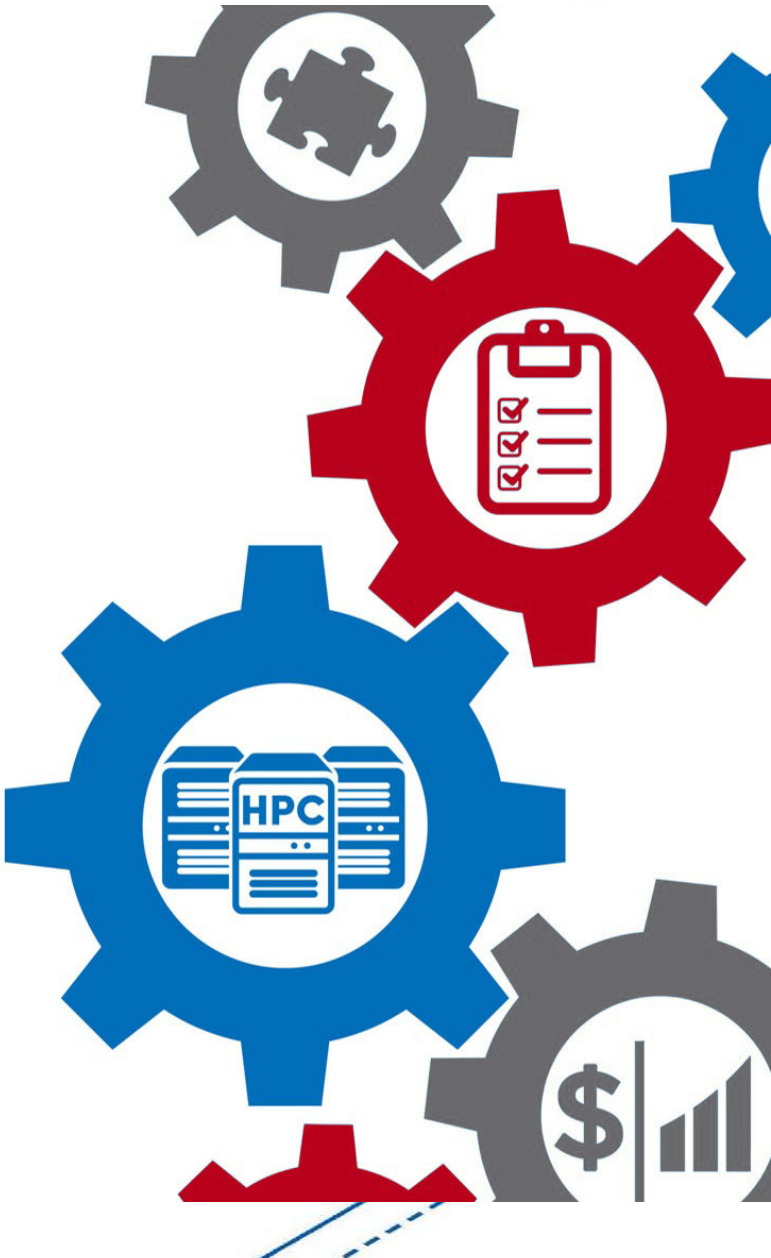
Includes:

- 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

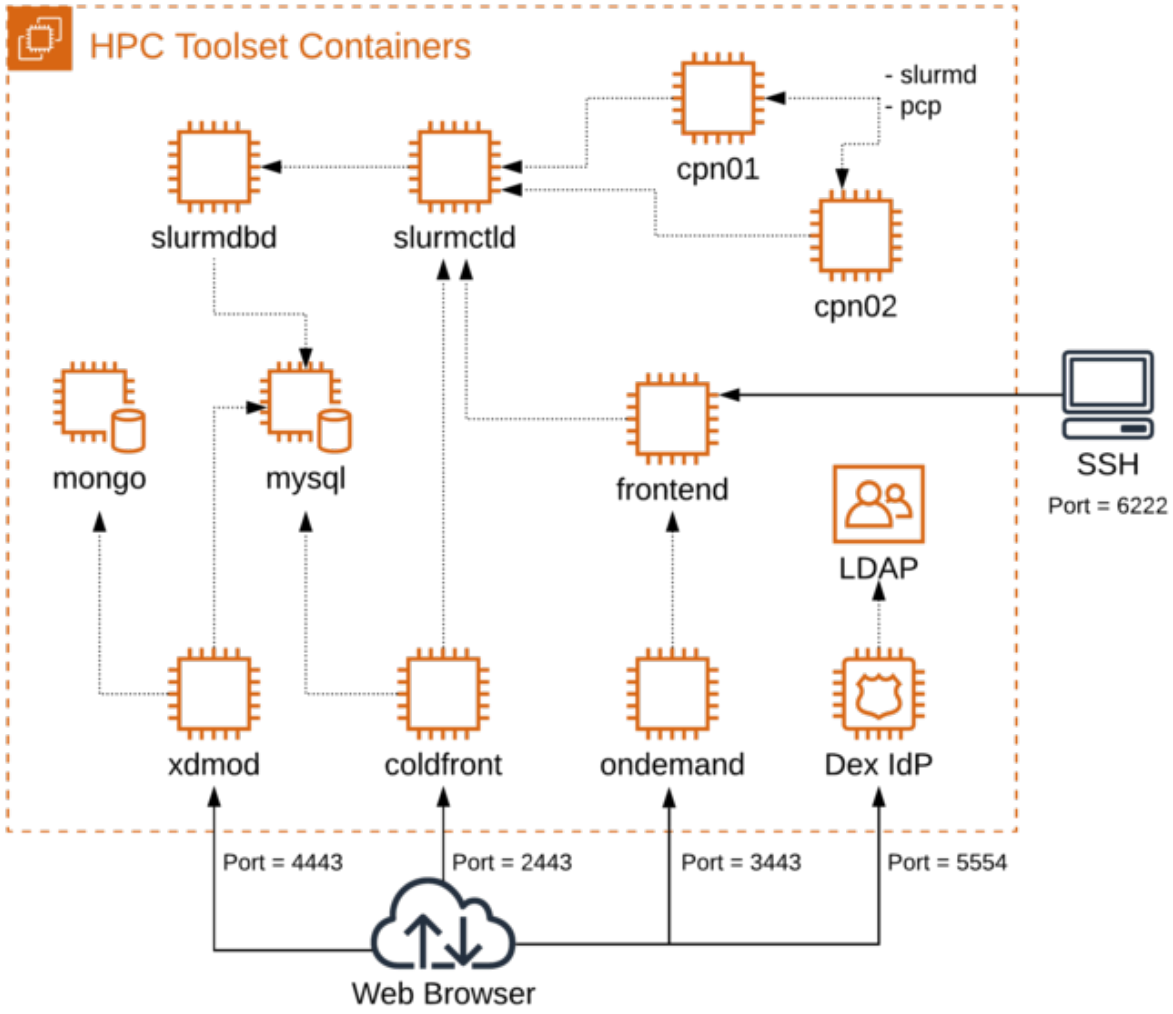


Open XDMoD – Usage & Performance Metrics

- 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 ~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.

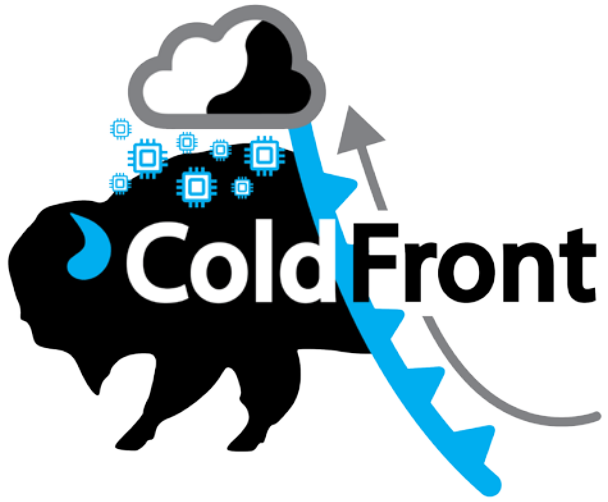
WARNING!!! DO NOT run these containers on production systems. This project is for educational purposes only. The container images we publish for the tutorial are configured with hard coded insecure passwords and should be run locally in development for testing and learning only.

Tutorial Walk Through

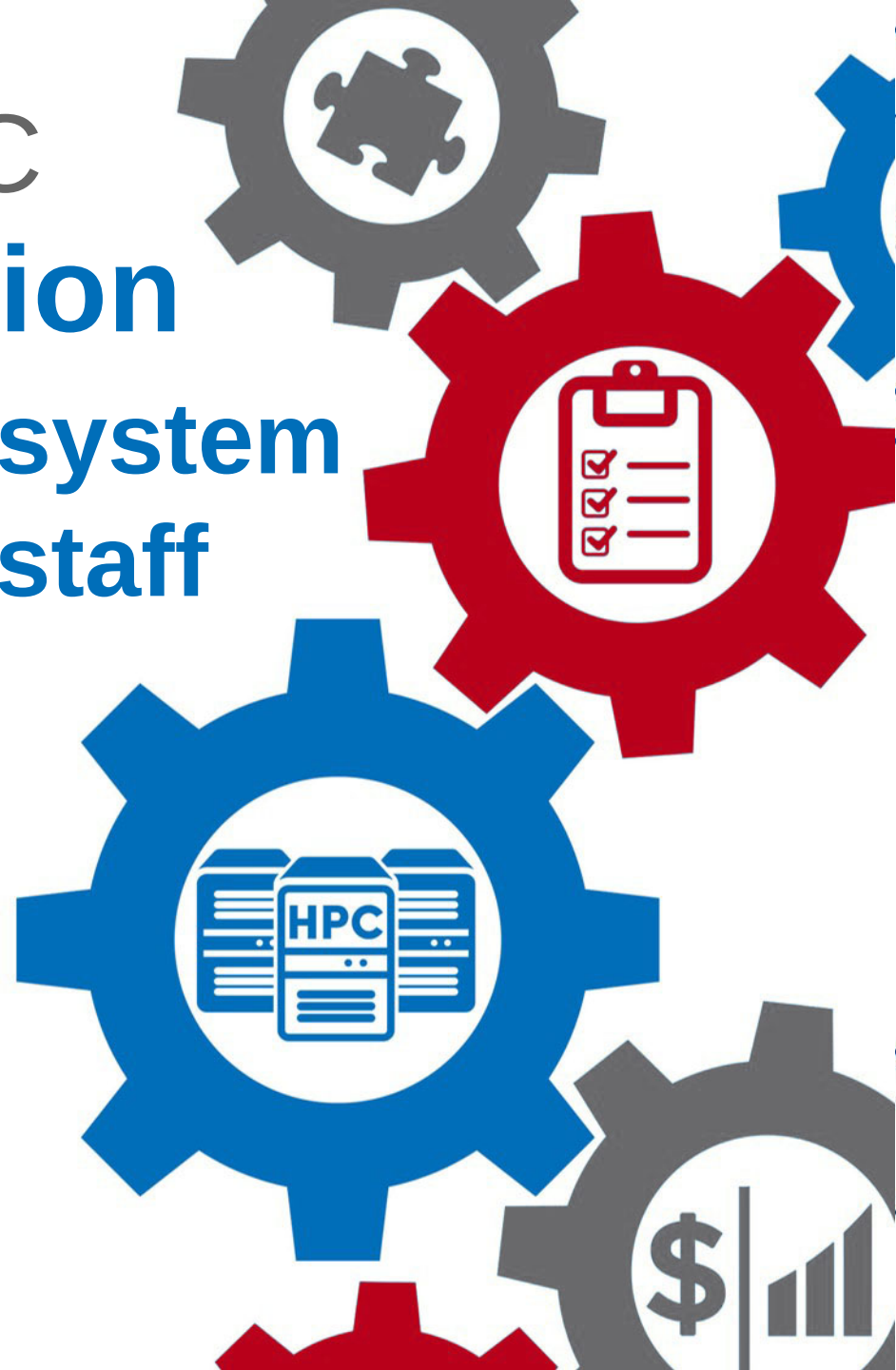
https://github.com/ubccr/hpc-toolset-tutorial

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



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



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Dori Sajdak, UB

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Automate access to your HPC resources

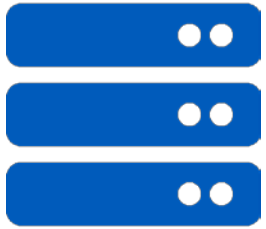
Manage access to all your resources in one place

Users

Policies

Databases

ACLs



Servers & Clusters

Cloud

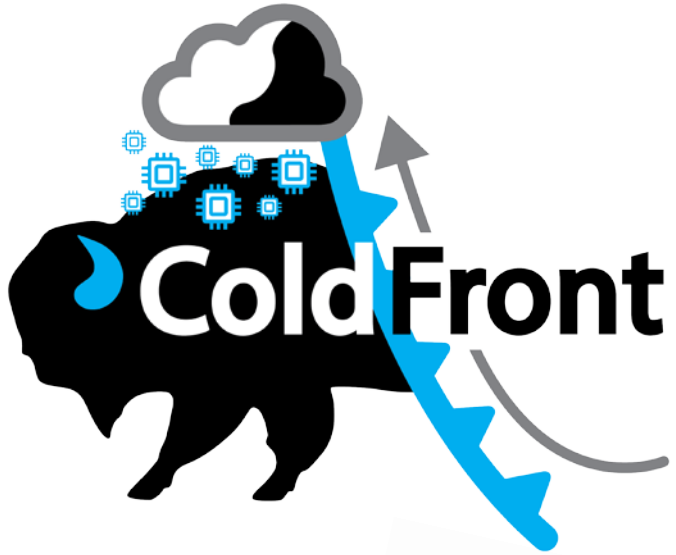
System Administrators

Software Licenses

Scientific Instruments

Storage

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
- Resources have attributes
  - Some might enforce limits:
    - storage (GB),
    - software (seats),
    - cloud (subscriptions)
  - Some might restrict access & may tie to plugins:
    - Is the resource private or public? Available only to certain users/groups?
    - Cluster config options – Slurm plugin
    - System access restricted by UNIX group? - FreeIPA plugin
    - Warranty expiration dates
- These attributes are customizable
- The attributes set on resources are inherited by allocations

Allocations

- Determines what resource an account has access to
- Allocations have start & end dates, creation & last modified dates, status, description, associated resource(s) & require a justification
- Allocations have attributes like resources that may set limits, restrict access, and/or tie into the ColdFront plugins. Examples include:
  - CPU/core hours
  - Scheduler account name
  - UNIX group
  - Storage quota
- Like Resource attributes, these are customizable
- Users emailed when expiration dates approach – configurable time spans
- Resource access can be removed when an allocation expires using ColdFront plugins
- Allocation Change requests NEW

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

Allocation Requests & Change Requests Can be Viewed by System Administrators

Allocation Requests

For each allocation request below, there is the option to activate the allocation request and to view the allocation's detail page.

By default, activating an allocation will make it active for 365 days.

#	Requested	Project Title	PI	Resource	Project Review Status	Status	Actions
2449	Apr. 28, 2022	Computational and Data Science and Engineering	Eric Walker (ericwalk)	UB VPN Access (Software License)	✓	Approved	Approve Details
2438	Apr. 21, 2022	Sunstar	Patricia Diaz (pidiazmo)	UB VPN Access (Software License)	✓	New	Approve Details

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
3	Apr. 06, 2022	Evolution of genomes with a focus on structural v...	Omer Gokcumen (omergokc)	ProjectStorage (Storage)		Approve Details
7	May. 02, 2022	Nonadiabatic dynamics in solar energy materials: ...	Alexey Akimov (alexeyak)	ProjectStorage (Storage)	30 days	Approve Details

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 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*

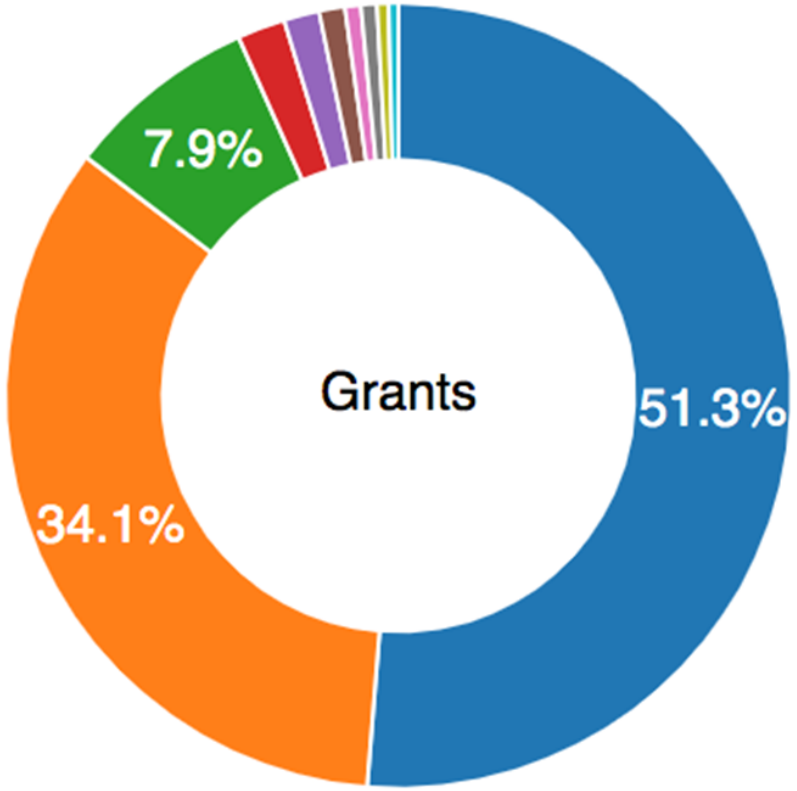
If you have no new information to provide, you are required to provide a statement explaining this in this box. Thank you!

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 Actions
My Test Project	May. 13, 2021	Dori Sajdak (djm29)	May. 13, 2021	May. 13, 2021		Mark Complete Email

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!**

slurm workload manager

OpenID

FreeIPA
Open Source Identity Management Solution

OPEN OnDemand

XDMoD
METRICS ON DEMAND

Vendor APIs

Integrations

Plug-ins (Django Apps)

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

Community Plugins:

OpenStack

Keycloak User Search

Starfish

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
- As PI users, request allocation change & allocation renewal
- Configure user with center director access & check out Project Review process
- Enable OnDemand integration

Contact Info:

Andrew Bruno - aebruno2@buffalo.edu

Dori Sajdak - djm29@buffalo.edu

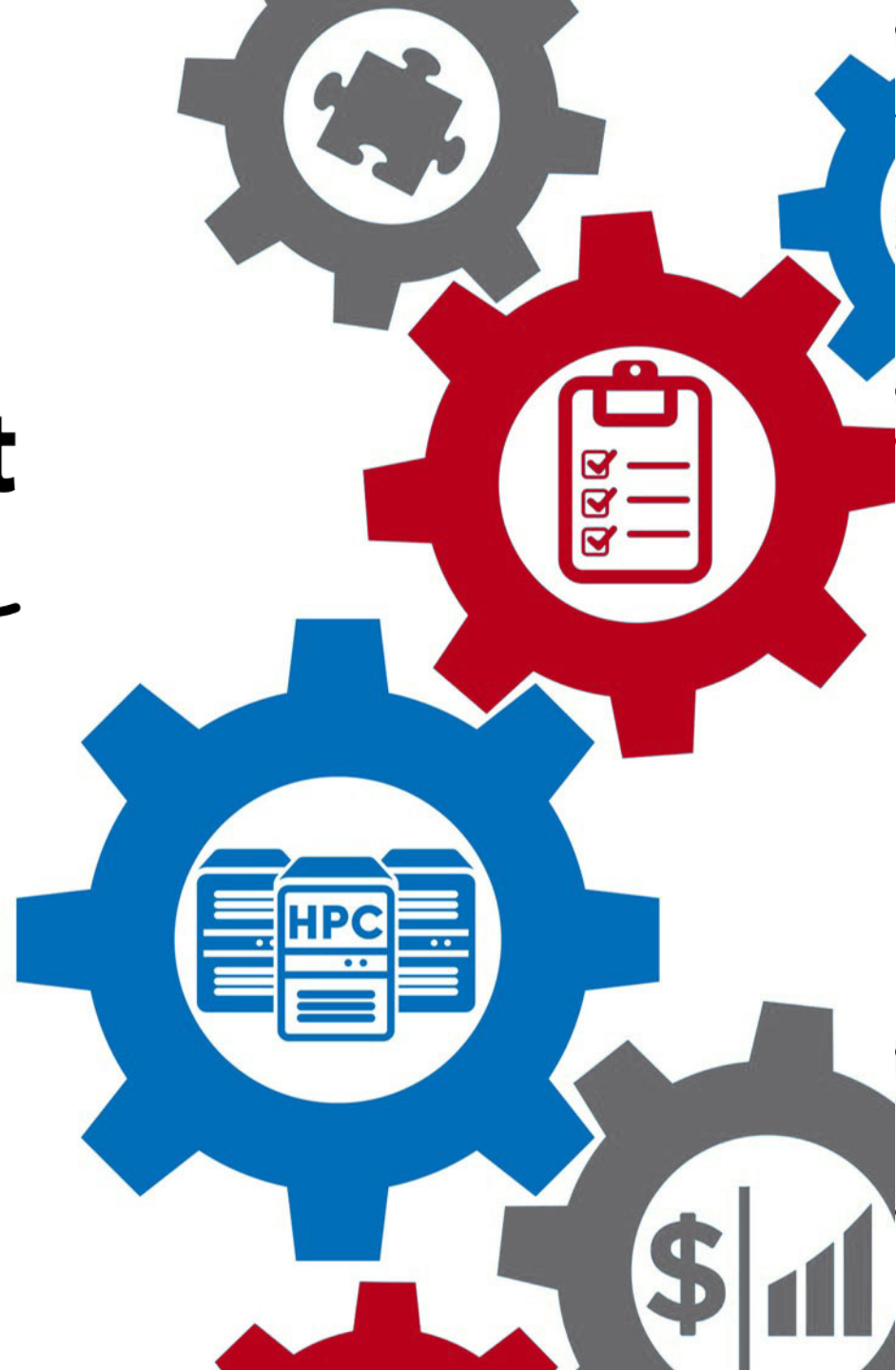
https://coldfront.io

More about UB CCR:

https://buffalo.edu/ccr

https://twitter.com/ubccr

ColdFront BOF:
Thursday, 7/14 9-10am
Arlington



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

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

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

NOW: Break: 90 minutes
Startup again at 1:30pm
Coming Up!
Part 3: Open OnDemand install and configuration
PM Break: 3-3:30
Part 4: Open OnDemand interactive app configuration
Part 5: Dynamic Batch Connect Fields

Other Places You'll Find us at PEARC22:

Performance Optimization of the Open XDMoD Datawarehouse - **best full paper!** Tues, 7/12 10:30-11am

Open OnDemand User Group Meeting: Tues, 7/12 1:30-2:30pm

Open XDMoD BOF: Wed, 7/13 1:30-2:30pm

Enhancing User-centric Workflows and Democratizing Access to Novel Advanced Research Computing BoF, Thur 7/14 8-9am

ColdFront BOF: Thur, 7/14 9-10am

OPEN OnDemand

Open, Interactive HPC via the Web

Alan Chalker, OSC

Travis Ravert, OSC

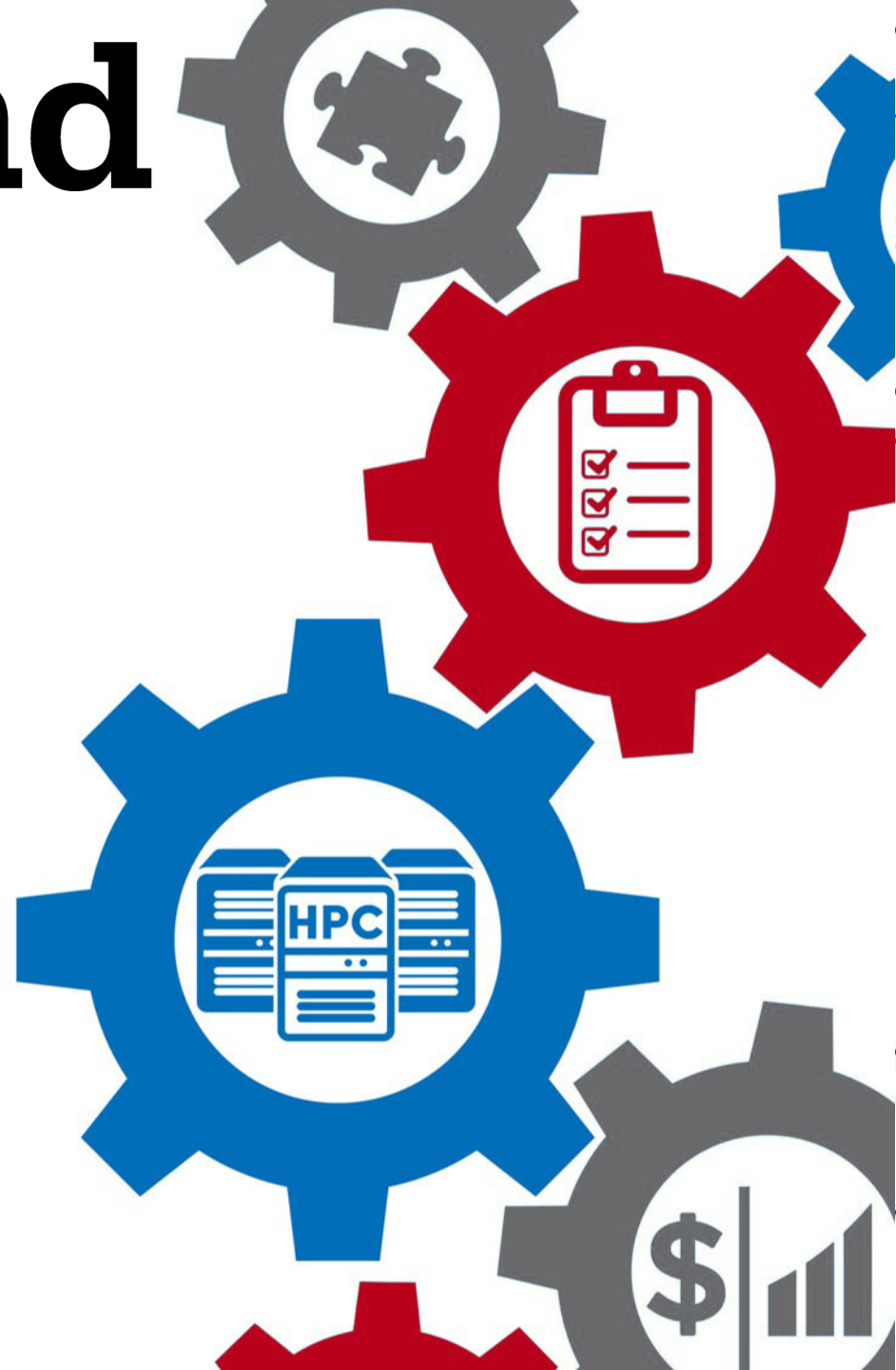
Trey Dockendorf, OSC

Jeff Ohrstrom, OSC

Bob Settlage, VT

Gerald Byrket, OSC

Open OnDemand is looking for contributors in the community. If interested, please speak with one of the OOD Team Members mentioned in this slide.



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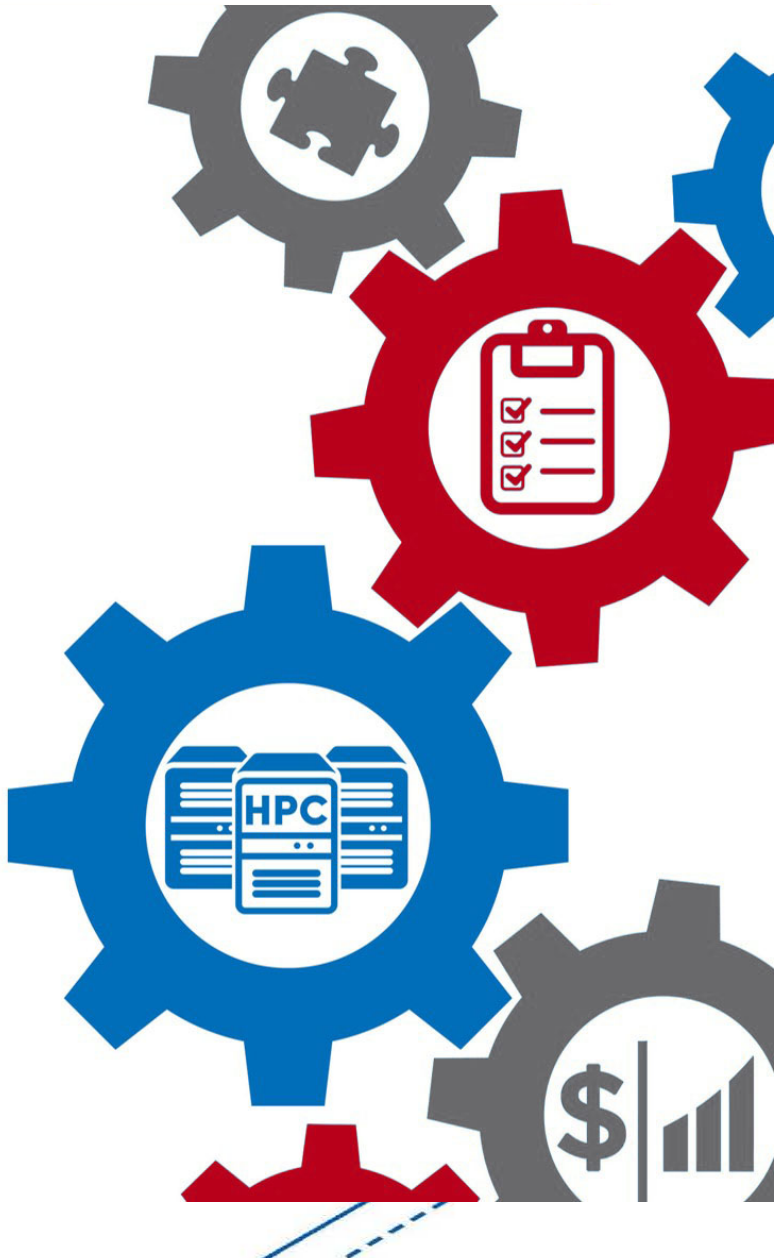
Introduction to Open OnDemand

Alan Chalker - OSC



OPENONDEMAND.ORG

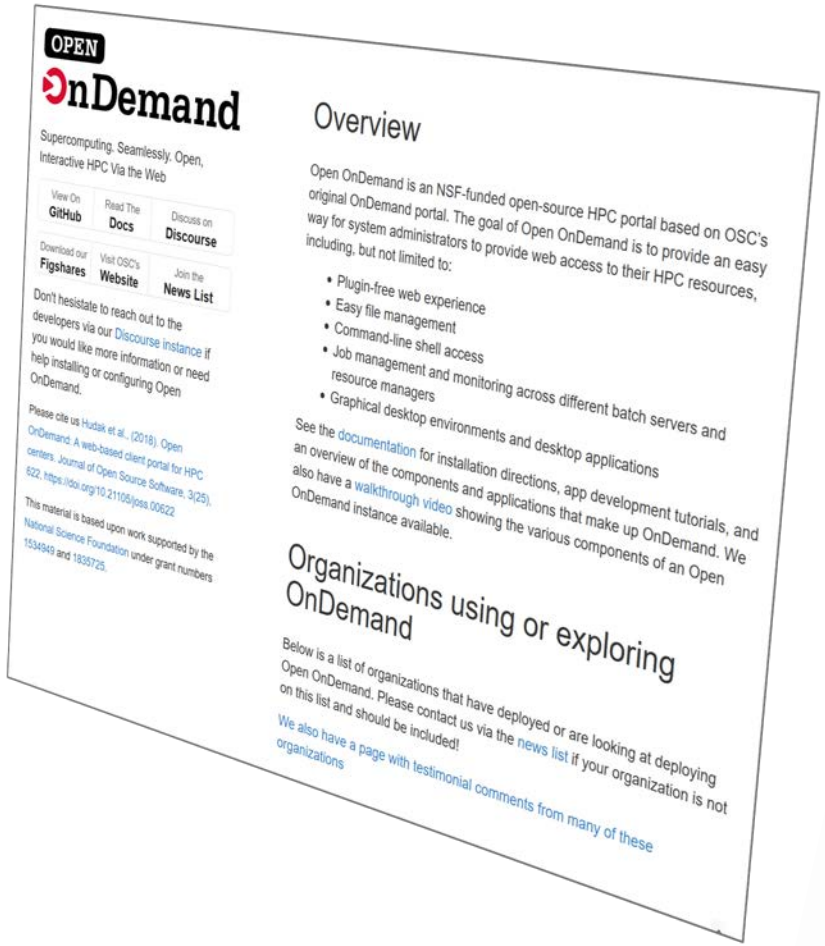
Use our Discourse instance for help

Join our mailing list for updates

Join our Monthly Open Office Forum

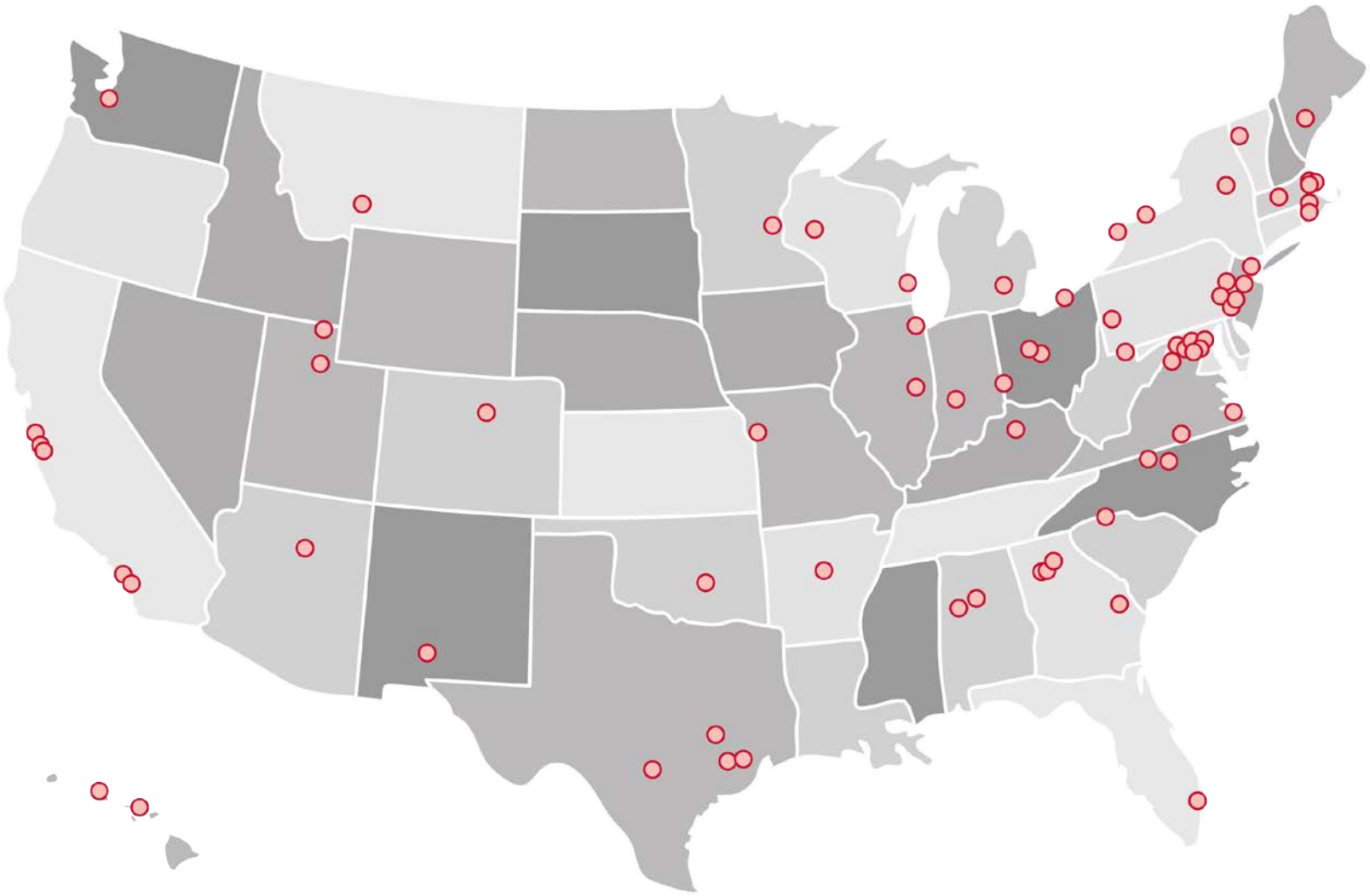
Join our Monthly Tips & Tricks Forum.

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

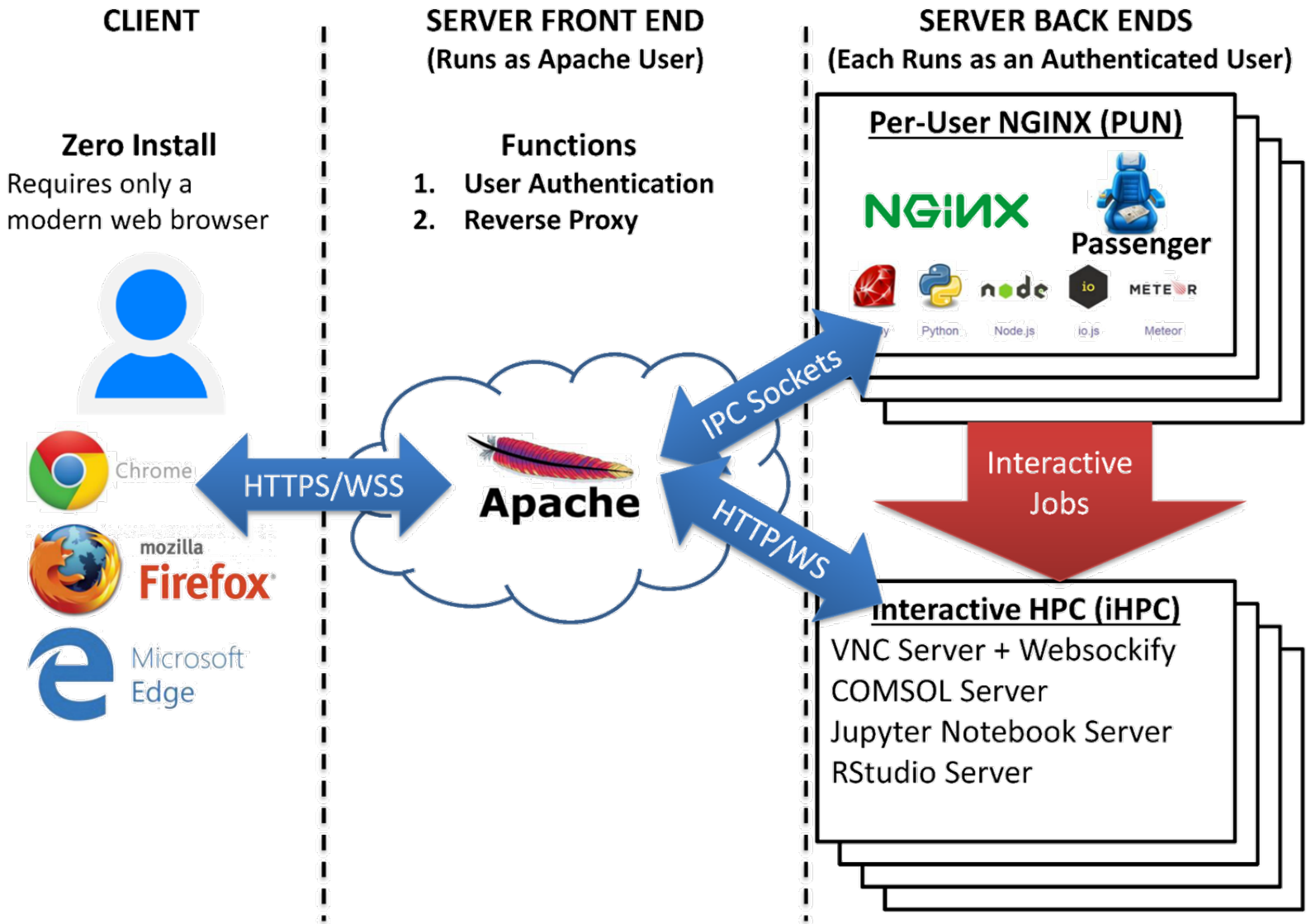
Example Current Engagements and Deployments

In Process of Installing

Cincinnati Children's
Colorado School of Mines
Federal Reserve Bank of San Francisco
جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology
MGHPCC Massachusetts Green High Performance Computing Center
Naval Nuclear Laboratory
Oak Ridge National Laboratory
The Ohio State University
Oregon State University
TOTALSIM US
UMassAmherst
University of Missouri
University of Hawai'i System
University of Hull
University of Kentucky
University of Maryland
UTSA The University of Texas at San Antonio
University of Washington
Washington University in St. Louis
X-ISS

Production Deployments

Arizona State University
Boston University
Caltech
Case Western Reserve University
Florida State University
Harvard University
Idaho National Laboratory
Illinois NCSA | National Center for Supercomputing Applications
Johns Hopkins University
Ohio Supercomputer Center
Michigan State University
Mississippi State University
NOR-TECH People Friendly Technology
Northern Arizona University
Old Dominion University
Berkeley
LSU
PennState
Pittsburgh Supercomputing Center
Princeton University
Purdue University
Roswell Park
Lafayette College
Rutgers
university of groningen
SMU
Stanford
Tandy Supercomputing Center
Shanghai Jiao Tong University
South Dakota State University
The University of Vermont
TRUBA
Texas A&M University
TCNJ The College of New Jersey
Seattle Children's
University at Buffalo
The University of Arizona
University of Houston Clear Lake
The University of Alabama at Birmingham
Vanderbilt University
The University of North Carolina at Chapel Hill
University of Oregon
University of Virginia
Virginia Tech
University of Central Oklahoma
University of Pittsburgh
The University of Utah
University of Michigan
Wageningen University & Research
Queen Mary University of London
Tufts University
The University of Tennessee Knoxville
Instituut Lorentz
Ghent University
UNSW Sydney
NVIDIA
SwRI Southwest Research Institute
University of Cincinnati
SDSC San Diego Supercomputer Center
Yale
Wright State University


CLIENT
SERVER FRONT END
(Runs as Apache User)
SERVER BACK ENDS
(Each Runs as an Authenticated User)
Zero Install
Requires only a
modern web browser
Functions
1. User Authentication
2. Reverse Proxy
Per-User NGINX (PUN)
NGINX
Passenger
Python
Node.js
io.js
Meteor
Chrome
mozilla
Firefox
Microsoft
Edge
HTTPS/WSS
Apache
IPC Sockets
HTTP/WS
Interactive
Jobs
Interactive HPC (iHPC)
VNC Server + Websockify
COMSOL Server
Jupyter Notebook Server
RStudio Server

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!

If you have an idea or want to work on any of the features or bug fixes, please feel free to reach out to us and we will get you started. We always want to include our community in the Open OnDemand efforts.

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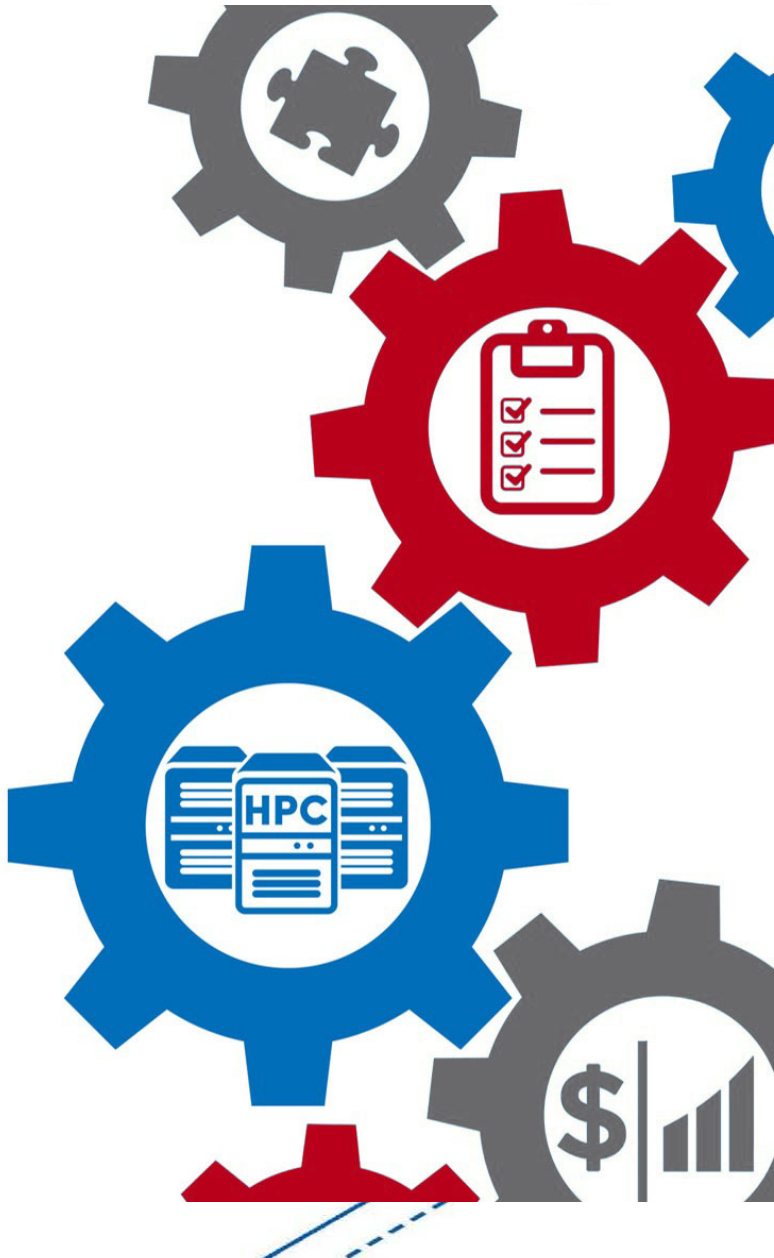
Customizing the OnDemand Dashboard

Gerald Byrket - OSC



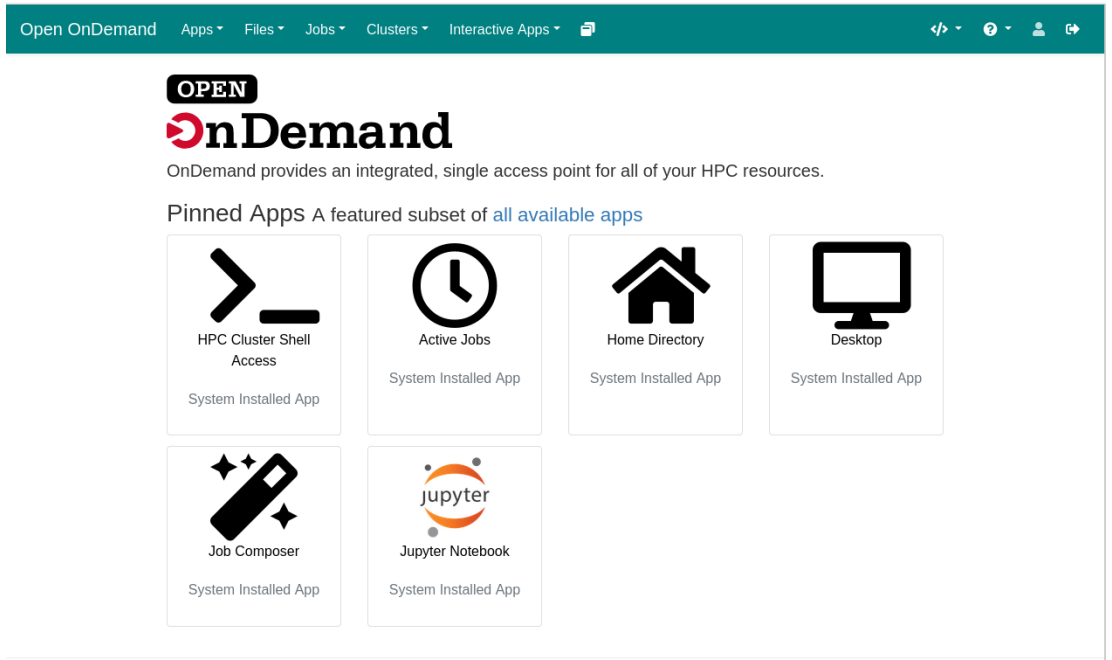
Hands on Tutorial: Dashboard in Development Mode

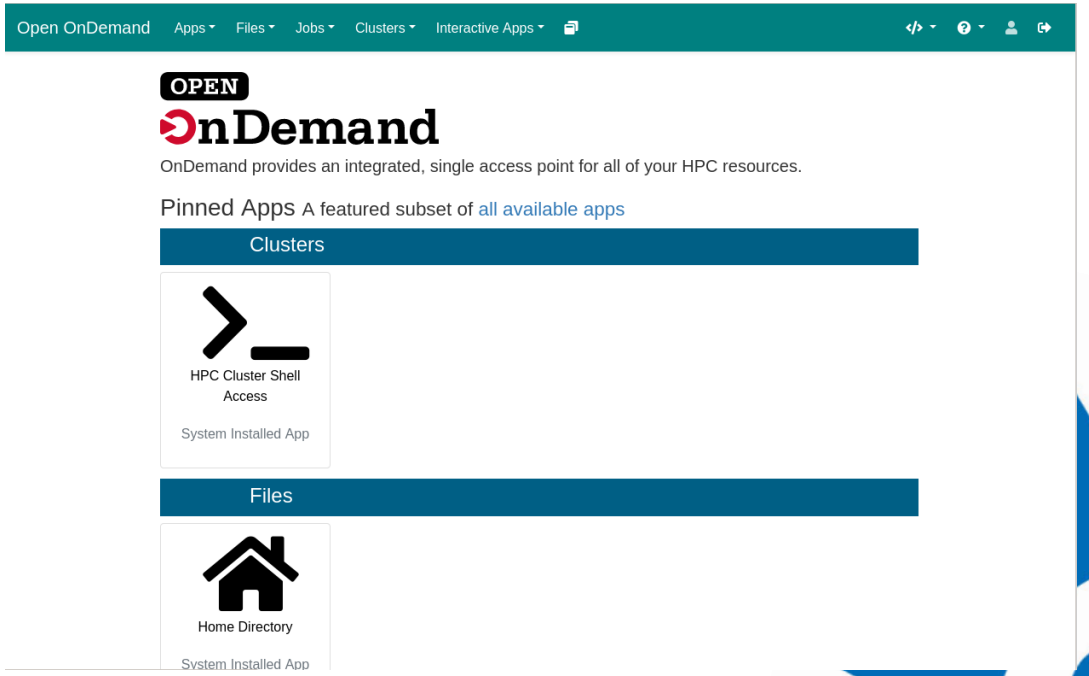
It Covers:

- **Setting up the dashboard in development mode**
- **Changing the navigation bar color**
- **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**

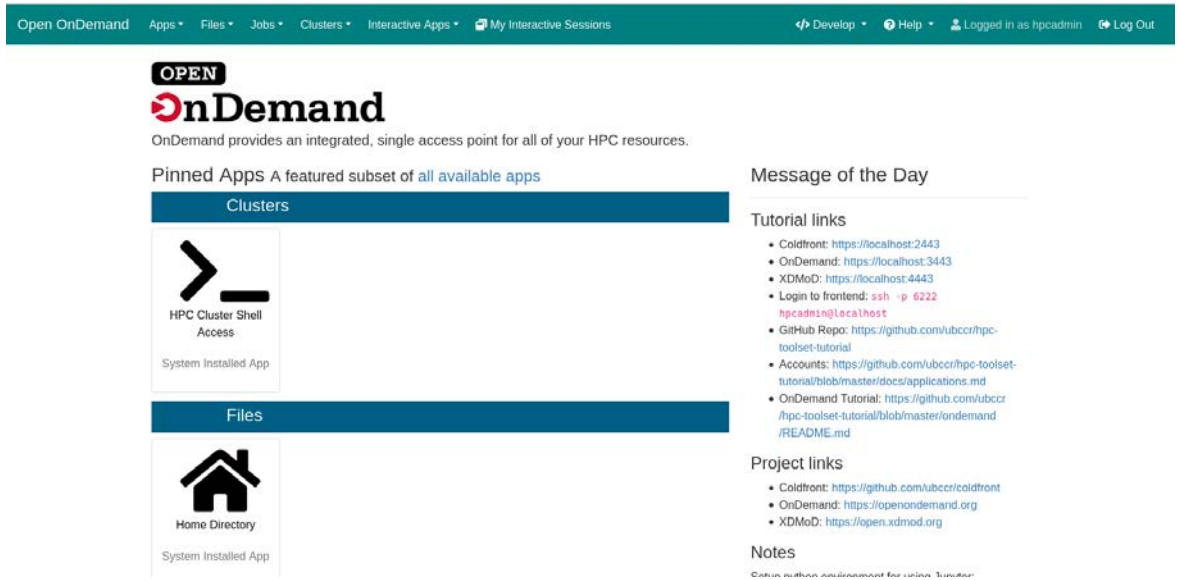




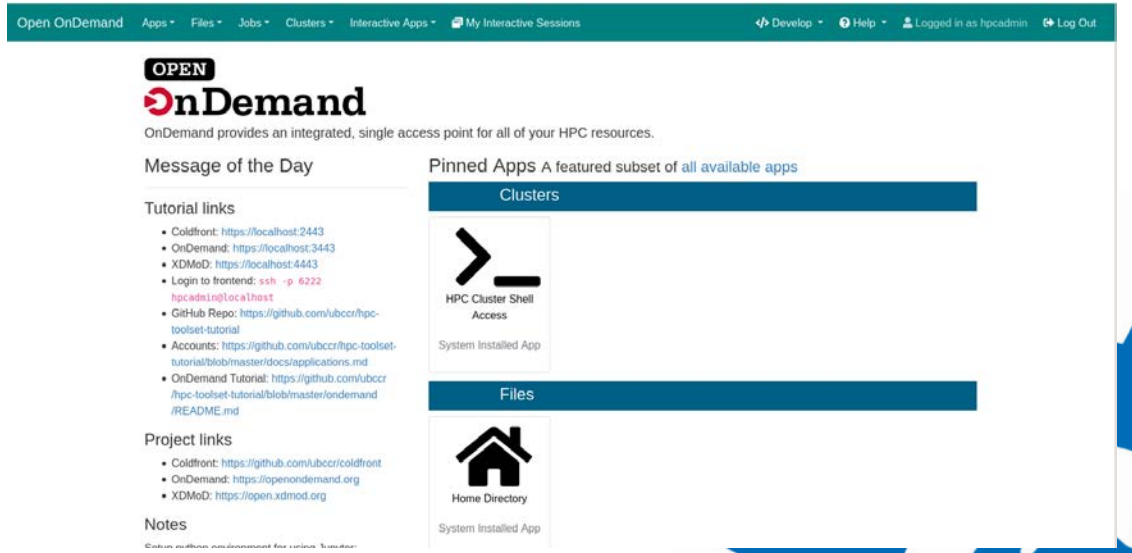
Dashboard Tutorial: Changing the layout

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

Before

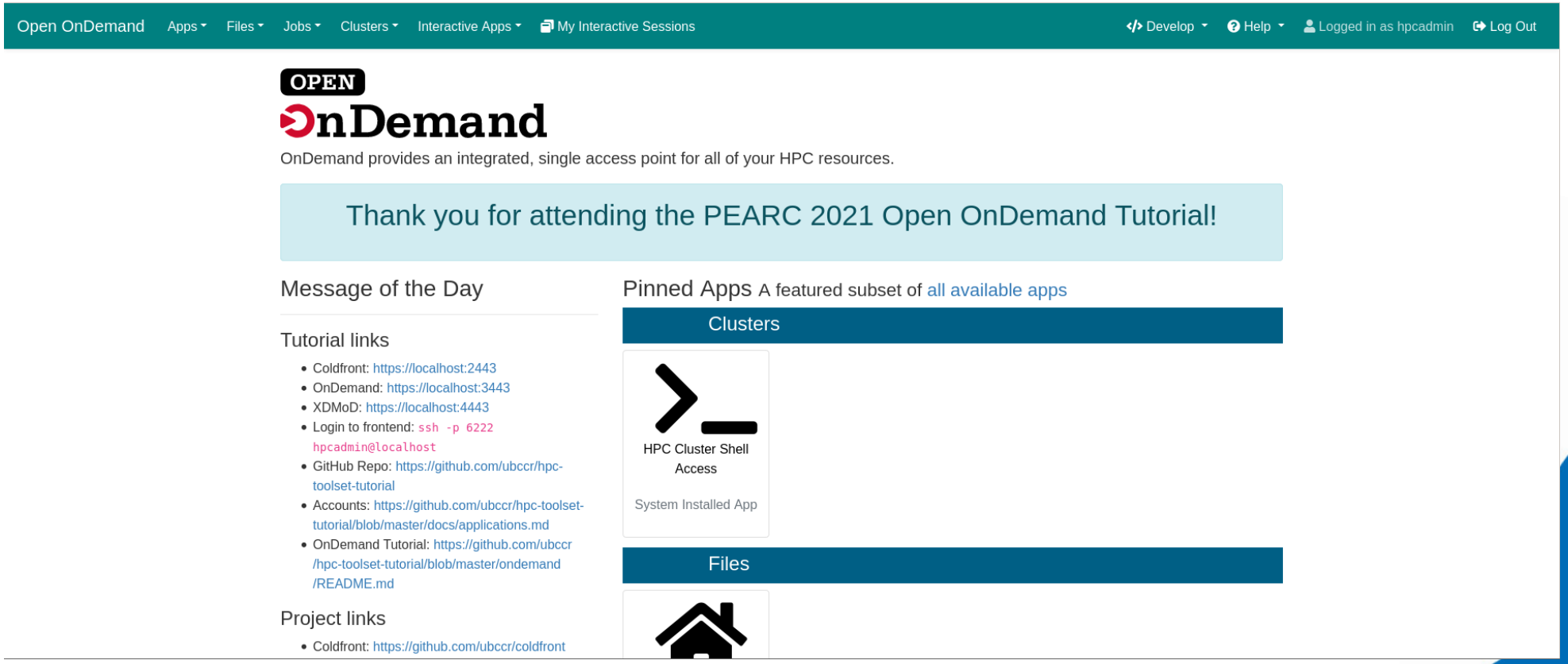


After



Dashboard Tutorial: Adding a new widget

- **Add a new custom widget**



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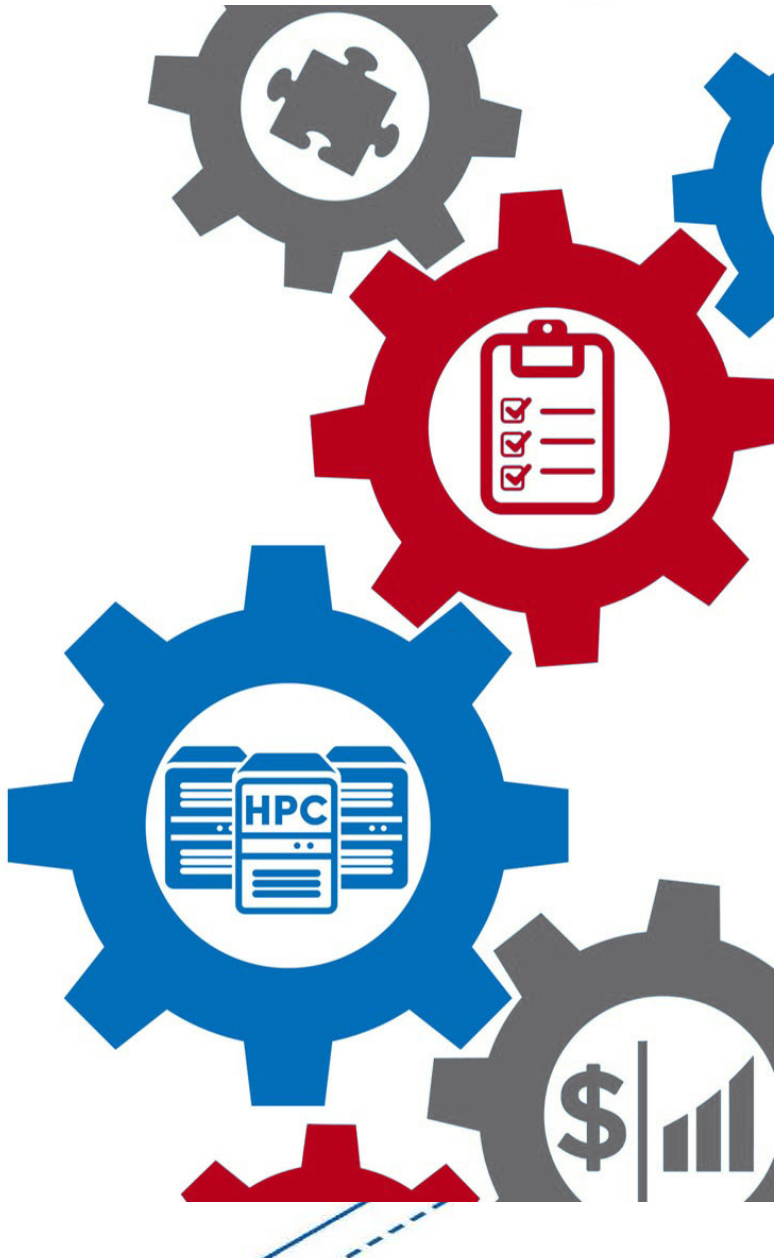
Create a Jupyter “Interactive App Plugin”

Travis Ravert - OSC



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

It Covers:

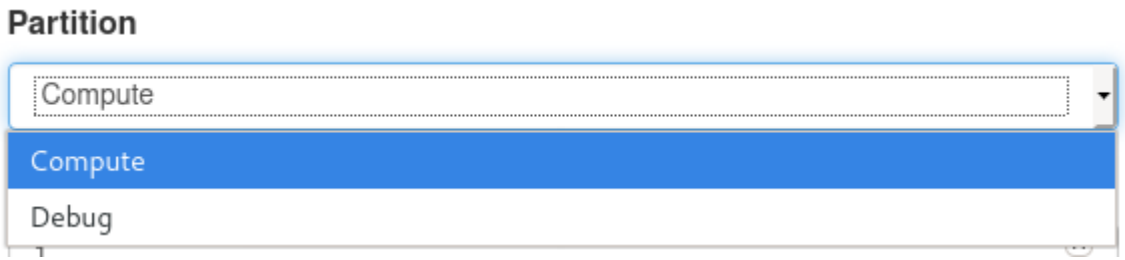
- **Getting the app to work.**
- **Checking logfiles to debugging failures.**
- **Changing the types of form items**
  - **From text input to select widgets**
- **Adding new form options**
- **Using Native scheduler options**
- **Explanations of files**
- **Promoting the app to production**

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**

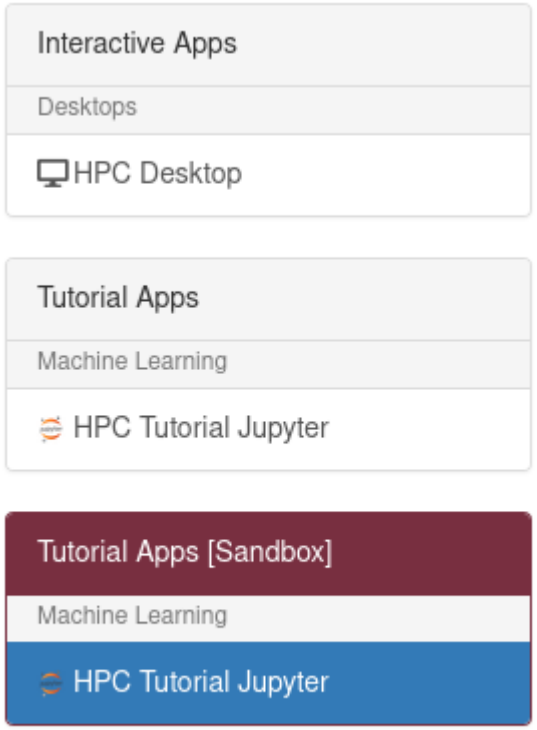
Jupyter Tutorial: Modify the Partition

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



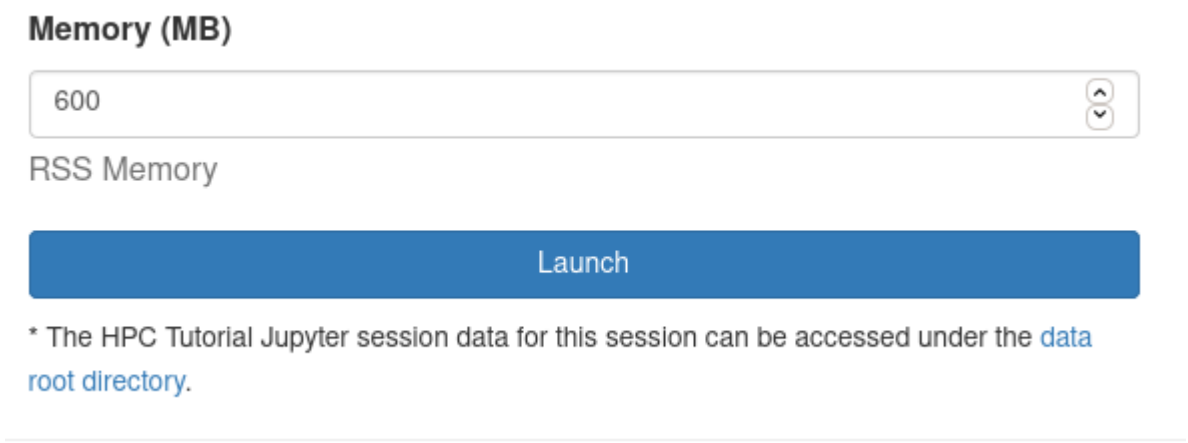
Jupyter Tutorial: Deploy to production

- **Deploy the app to production for other users**



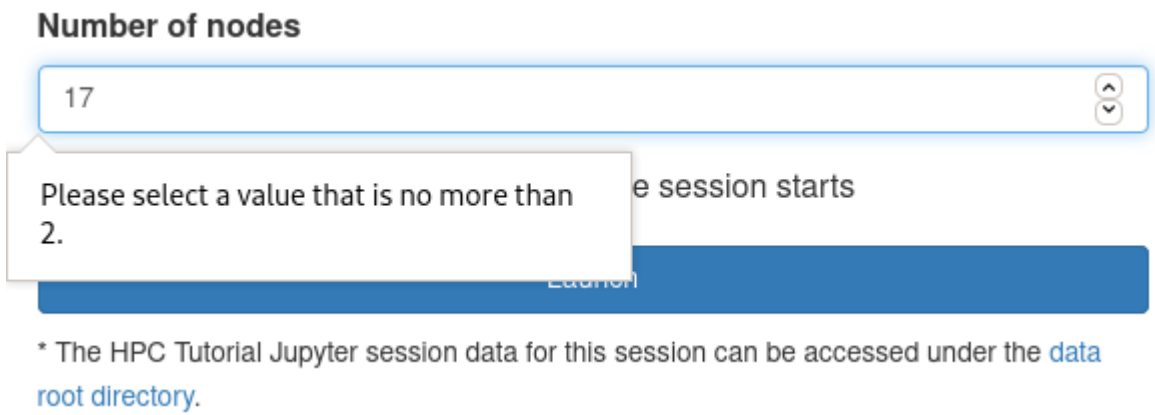
Jupyter Tutorial: Set the memory request for the job

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



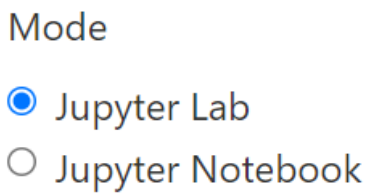
Jupyter Tutorial: Limit the number of nodes

- **Put an upper limit on the number of nodes allowed**



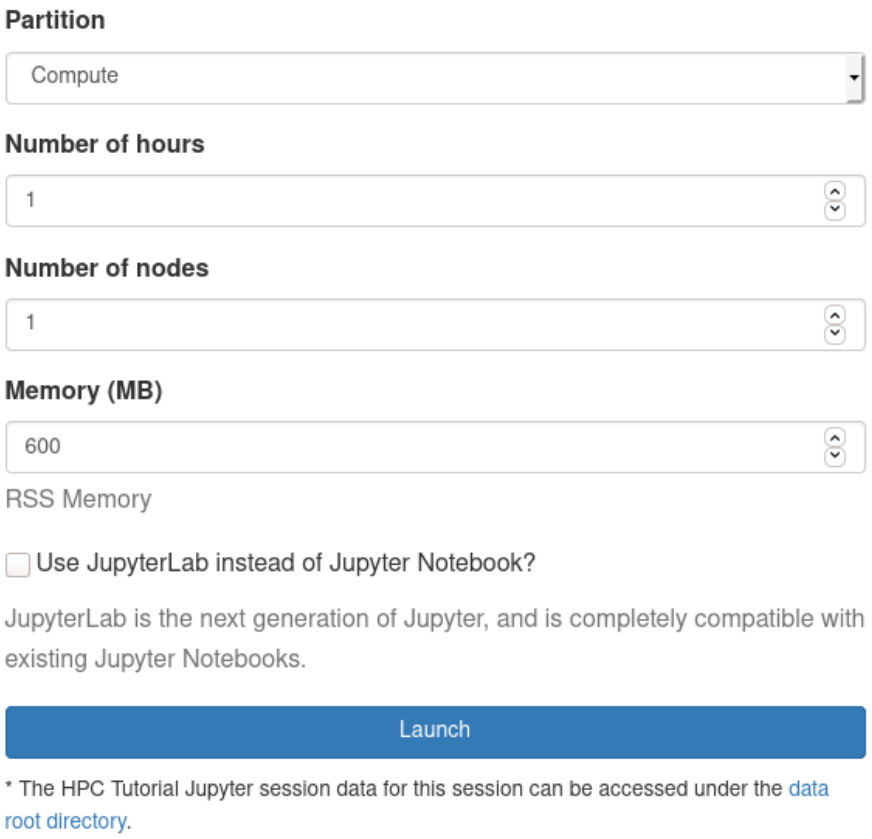
Jupyter Tutorial: Add a radio button to start JupyterLab

- **Add radio buttons so users can boot JupyterLab or Jupyter Notebook**



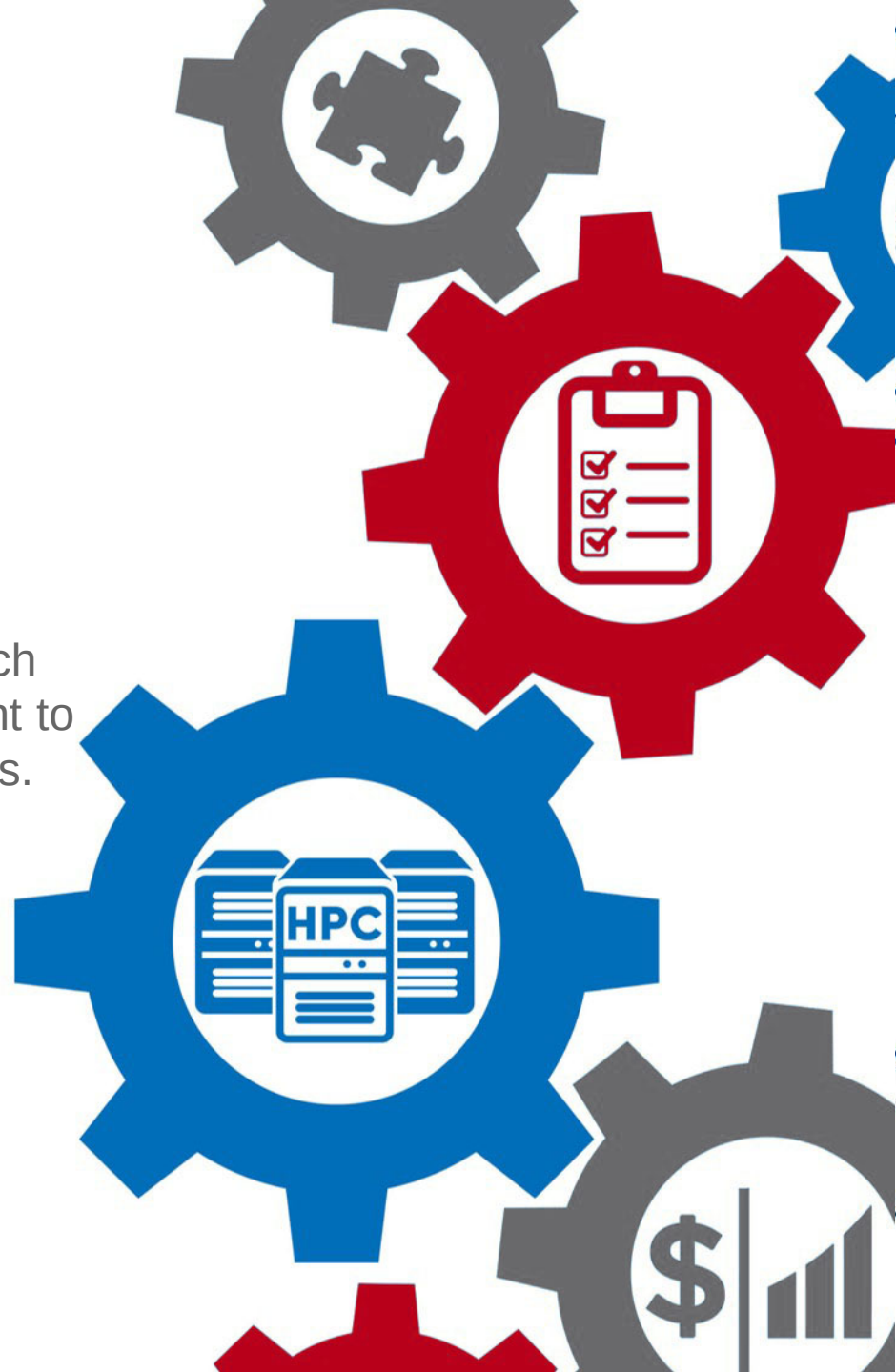
Jupyter Tutorial: Delete unused fields

- **Delete unused fields to clean up the form**



Break

If you have an idea or want to work on any of the features or bug fixes in OOD, please feel free to reach out to us and we will get you started. We always want to include our community in the Open OnDemand efforts.



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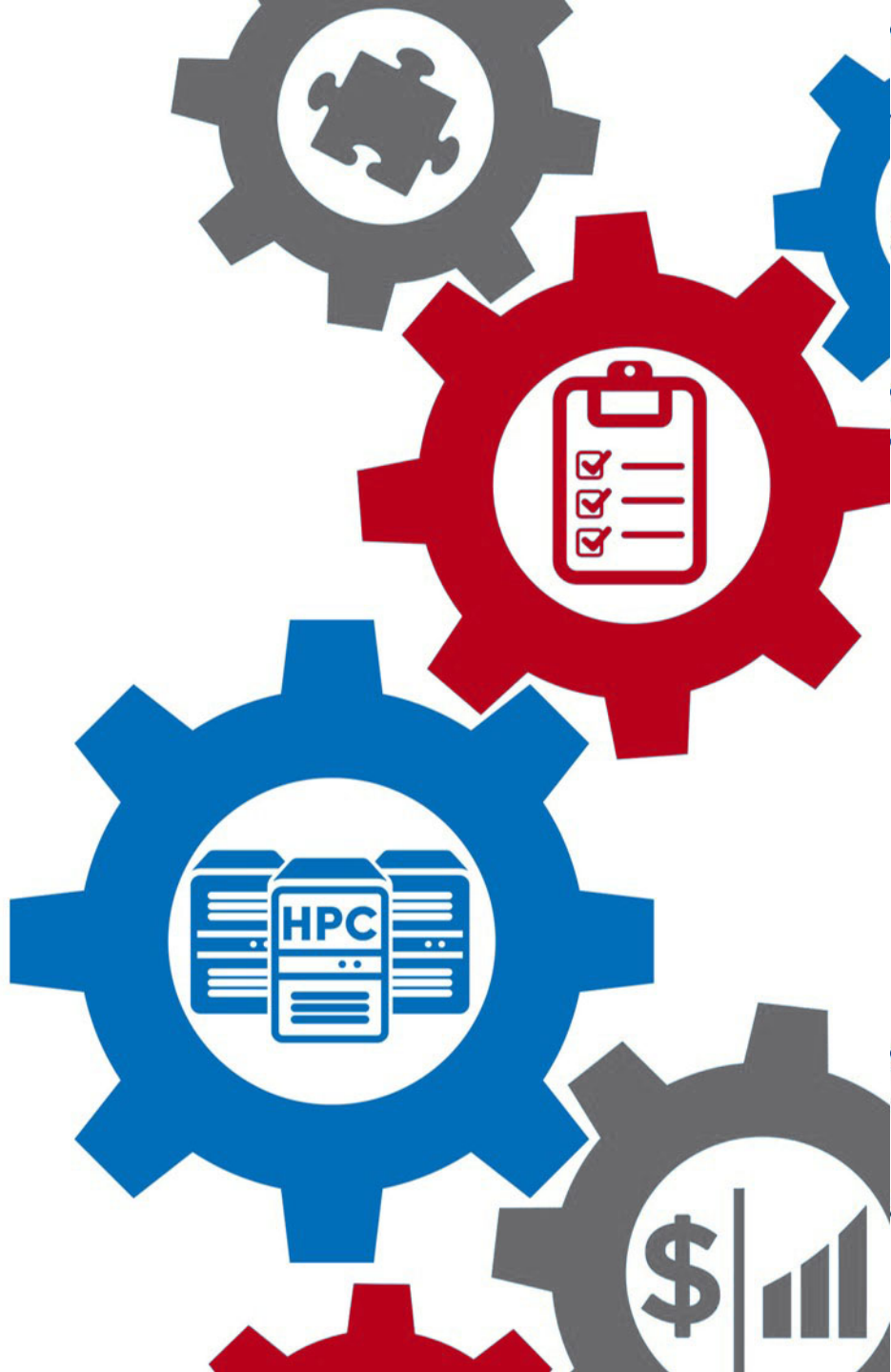
Dynamic Batch Connect Fields

Travis Ravert - OSC



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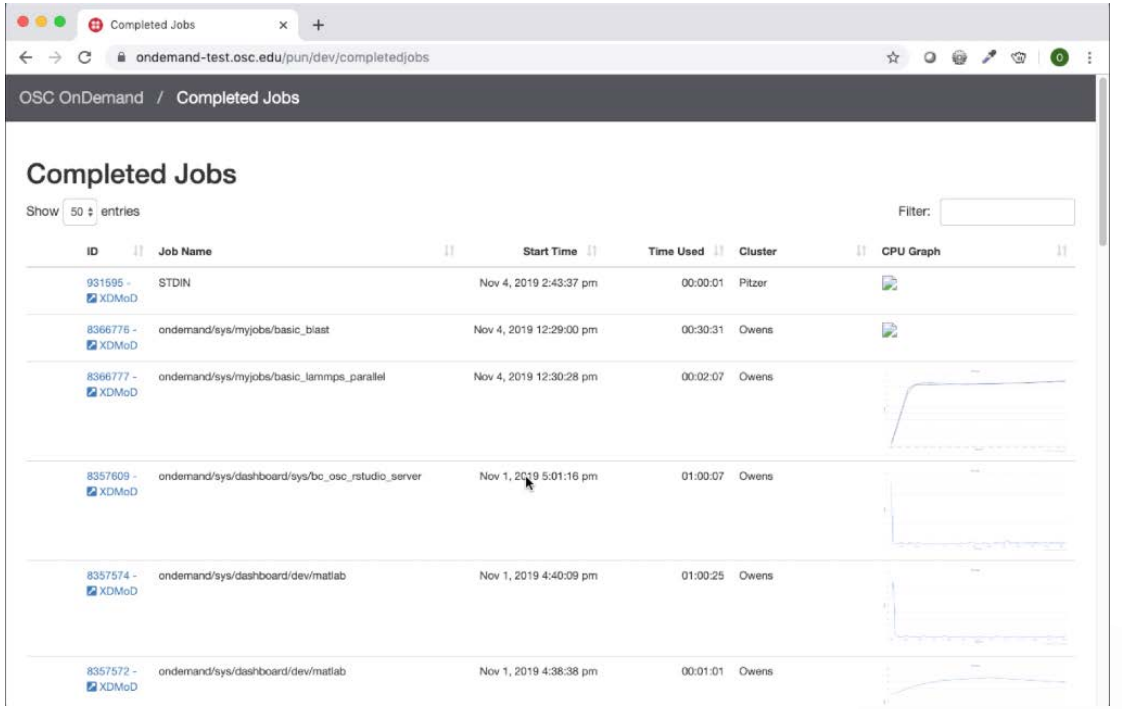
Future plans

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



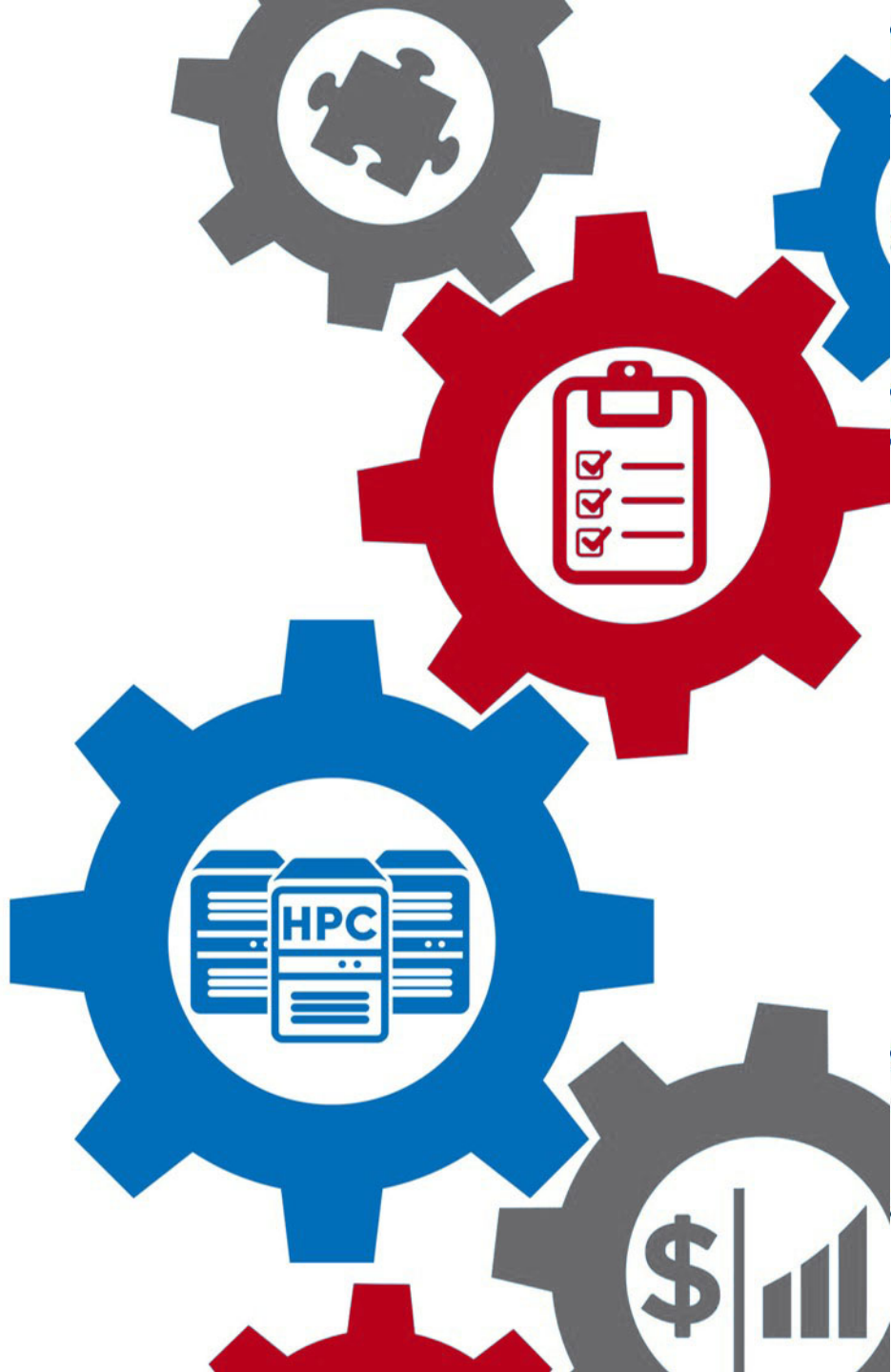
Find more ways to help users optimize their jobs!

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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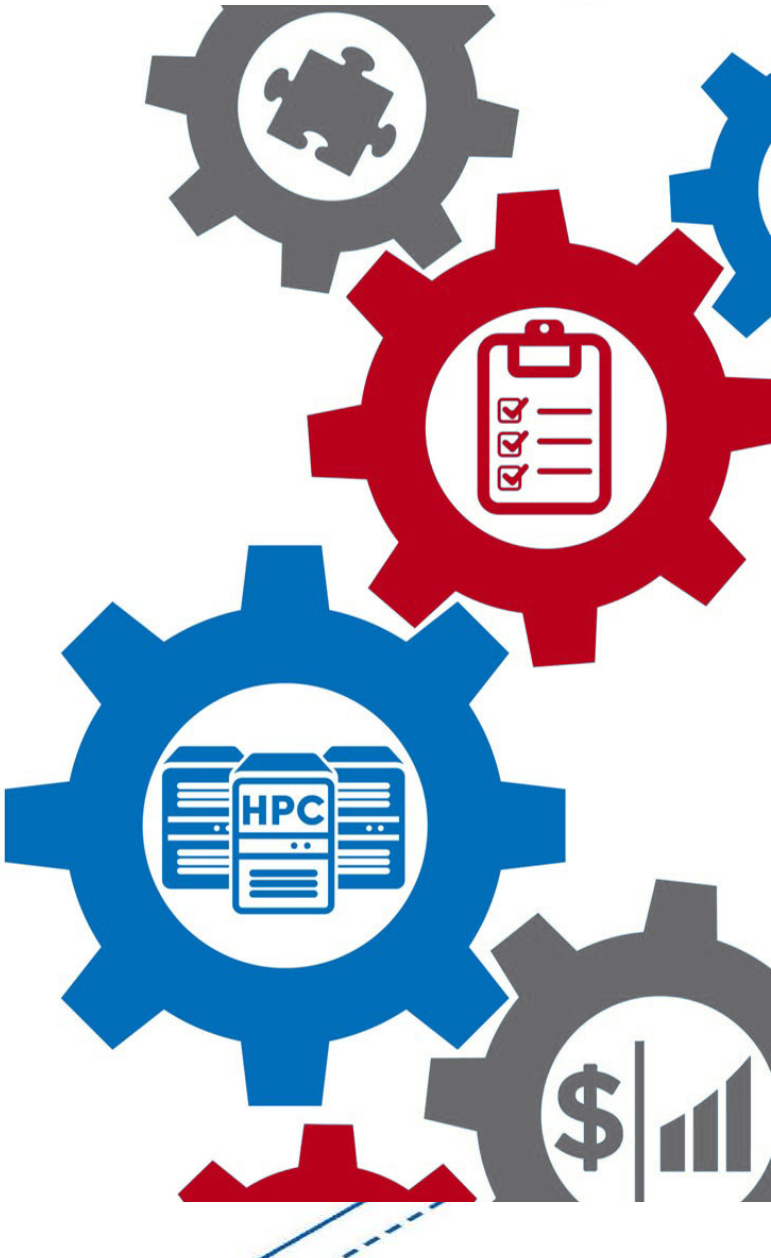
NSF Proposal Collaboration



Looking for smaller centers interested in working with us to get assistance on installing & managing these products

Contact Joseph White at UB
jpwhite4@buffalo.edu

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/

Other places you'll find us at PEARC22:

Performance Optimization of the Open XDMoD Datawarehouse - **best full paper!** Tues, 7/12 10:30-11am

Open OnDemand User Group Meeting: Tues, 7/12 1:30-2:30pm

Open XDMoD BOF: Wed, 7/13 1:30-2:30pm

Enhancing User-centric Workflows and Democratizing Access to Novel Advanced Research Computing BoF, Thur 7/14 8-9am

ColdFront BOF: Thur, 7/14 9-10am

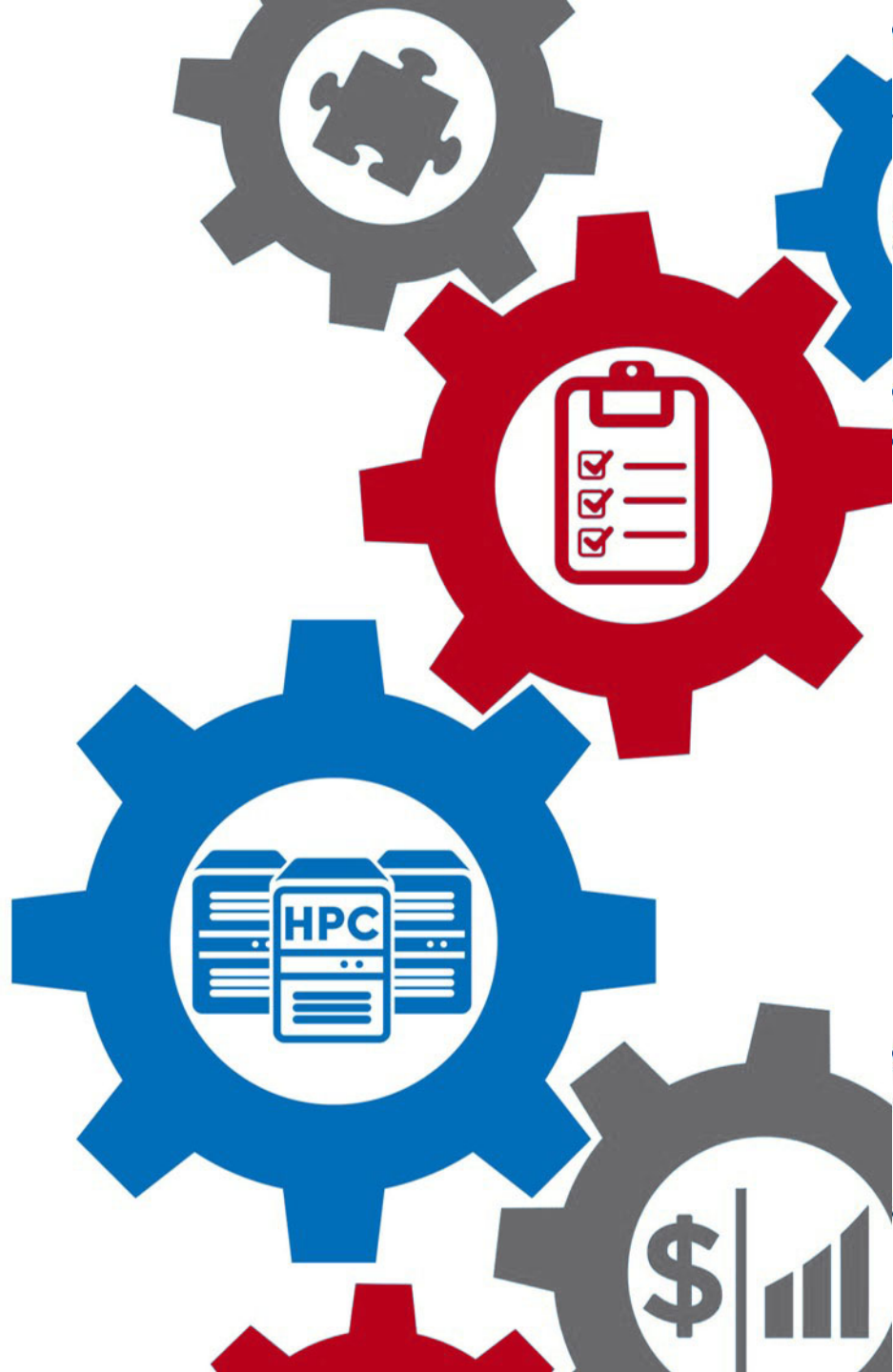
Visit us at the OnDemand table in the vendor area too!

Staff may be available after workshop concludes for specific questions. Please also join us on Slack!

Thank you for attending!

Please fill out the post-tutorial survey

We value your opinions!



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