

— **OPEN**

 **nDemand**

Open
OnDemand
Quarterly
SCAG

Aug 25, 2020



Ohio Supercomputer Center



University at Buffalo

Center for Computational Research



State of the state

- Community comments/thoughts/concerns?
- Burning app needs?

New collaborations/projects

- Harvard IQSS voicing interest in contributing development time to improvement of UX
- Globus interested in working with us for integration and offering developer time to help
- Active discussion with Joe Stubbs and Steve Black from TACC regarding possibly adopting of and contributing to resource and application definition standards being developed between TACC, IU, others (follow up from PERAC)
- Started talking with Airavata/SciGap team to build a prototype integration between OnDemand and Airavata

PEARC20 takeaways

- Lots of positive feedback to tutorial
- Lots of interest
- Lots of sites using/installing it that are/were not represented on our known slides
- Support of Gateways and pipelines/workflow is important and being hobbled together at multiple sites

1.8 Release

<https://osc.github.io/ood-documentation/latest/release-notes/v1.8-release-notes.html>

- Features:
 - XDMoD reports and links – Dashboard and Job Composer – slide 6/7
 - App submit to multiple clusters - slide 8
 - Retain completed jobs panel for debugging -- slide 9
 - **dd (dynamic) information to job panel (info.html.erb) -- slide 10**
 - DEX is default authenticator
 - Chrome noVNC copy/paste patch
 - VS code server app

1.8 Release: XDMoD Reports and Links

OSC OnDemand Files Jobs Clusters Interactive Apps Help Develop Help Logged in as efranz Log Out

Ohio Supercomputer Center
An OH-TECH Consortium Member

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

Message of the Day

2020-07-31 - Backup failures for Project on August 1st and 2nd
OSC experienced backup failures on our GPFS file systems (both Project file systems, /fs/project and /fs/ees) the mornings of August 1st and 2nd. The underlying cause was identified and backups were operating as expected the morning of August 3rd. As a result of these failed backups, OSC will not be able to complete some file restore requests for files changed between approximately 2020-07-31 02:30 through 2020-08-02 02:30.

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 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 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/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:

Jobs Efficiency Report - 2020-07-25 to 2020-08-24
54.5% efficient 45.5% inefficient
15 inefficient jobs / 33 total jobs

Core Hours Efficiency Report - 2020-07-25 to 2020-08-24
18.8% efficient 81.2% inefficient
65.5 inefficient core hours / 80.7 total core hours

Recently Completed Jobs - 2020-07-25 to 2020-08-24

ID	Name	Date	CPU
11030363	ondemand/sys /dashboard	8/6	00.4
11025209	wlag/weld_predictor	8/5	00.4
14021	ondemand/sys /myjobs/default	8/5	N/A
14020	ondemand/sys /myjobs/default	8/5	N/A
10978802	ondemand/sys /dashboard	8/4	01.7
10974801	wlag/weld_predictor	8/3	01.9
10974800	wlag/weld_predictor	8/3	00.3
10936746	STDIN	8/3	00.3
10935957	ondemand/sys /myjobs/default	8/3	00.8
10935689	ondemand/sys /myjobs/default	8/3	00.6

Showing first 10 of 33 jobs. See your XDMoD dashboard for more information.

XDMoD Hello, Eric Franz (logout) Ohio Supercomputer Center My Profile About Roadmap Contact Us Help

Dashboard Usage Metric Explorer App Kernels Report Generator Job Viewer About

Job Efficiency Report - 2020-07-25 to 2020-08-24

Job Efficiency
Total Job Count: 33
Inefficient Job Count: 15

Core Hour Efficiency
Total Core Hours: 80.73
Inefficient Core Hours: 65.54

Wait Hours - 2020-07-25 to 2020-08-24

Wait Hours: Per Job {User = efranz} (green bars)
Std Err: Wait Hours: Per Job {User = efranz} (blue dots)

Jobs - 2020-07-25 to 2020-08-24

Job Identifier	Start	End	CPU
owens-11030363	2020-08-21 15:21:38	2020-08-21 16:15:15	00.4
owens-11025209	2020-08-20 17:03:52	2020-08-20 17:05:10	00.4
qp-14021	2020-08-20 10:27:05	2020-08-20 10:27:07	N/A
pitzer-exp-14020	2020-08-20 10:26:50	2020-08-20 10:26:53	N/A
owens-10978802	2020-08-19 10:45:04	2020-08-19 10:52:35	01.7
owens-10974801	2020-08-18 14:51:48	2020-08-18 14:53:01	01.9
owens-10974800	2020-08-18 14:51:17	2020-08-18 14:52:31	00.3
owens-10936746	2020-08-11 15:53:32	2020-08-11 17:54:31	00.3
owens-10935957	2020-08-11 11:24:53	2020-08-11 12:36:10	00.8
owens-10935689	2020-08-11 10:10:49	2020-08-11 11:11:32	00.6

Displaying 1 - 10 of 33

Wait times by queue - 2020-07-25 to 2020-08-24

Queue: datta-backfill-pa..., datta-backfill-se..., datta-parallel, datta-serial, debug, gpbackfill, gpbackfill-seria..., gpudebug, gpuparallel-48cor..., gpuparallel-quad

Wait Time Per Job (hours)



1.8 Release: XDMoD Reports and Links

The Job Composer interface displays a list of jobs under the 'Jobs' tab. A red arrow points from the 'XDMoD' link in the job details to the 'Accounting data' link in the search history.

Created	Name	ID	Cluster	Status
May 28, 2020 10:37am	(default) Simple Sequential Job		Pitzer	Not Submitted
May 28, 2020 10:34am	(default) Simple Sequential Job		Owens	Not Submitted
May 19, 2020 3:28pm	auto - Simple Sequential Job	10276299.owens-batch.ten.osc.edu - XDMoD	Owens	Completed
May 19, 2020 3:28pm	auto - Simple Parallel Job	10276298.owens-batch.ten.osc.edu - XDMoD	Owens	Completed
May 19, 2020 3:28pm	auto - Parallel job with MPI and OpenMP	10276297.owens-batch.ten.osc.edu - XDMoD	Owens	Completed
May 19, 2020 3:28pm	auto - MPI Hello World	10276296.owens-batch.ten.osc.edu - XDMoD	Owens	Completed
May 19, 2020 3:28pm	auto - Hello OpenMP World in C	10276295.owens-batch.ten.osc.edu - XDMoD	Owens	Completed
May 19, 2020 3:28pm	auto - Basic Star-CCM+ Serial Job - Owens	10276294.owens-batch.ten.osc.edu - XDMoD	Owens	Completed
May 19, 2020 3:28pm	auto - Basic Star-CCM+ Parallel Job - Owens	10276293.owens-batch.ten.osc.edu - XDMoD	Owens	Completed

Job Details

10276299.owens-batch.ten.osc.edu - XDMoD

Job Name: auto - Simple Sequential Job

Submit to: Owens

Account: Not specified

Script location: /users/PZS0562/efranz/ondemand/src/ondemand/apps/myjobs/data

Script name: sequential_t_job.sh

Folder Contents:

- basic_sequential.o10276299
- message.in
- message.out
- myscript.sh
- sequential_job.sh

The XDMoD Job Viewer interface displays detailed information for job 10276299. A red arrow points from the 'Accounting data' link in the search history to the 'Accounting data' tab in the job viewer.

Search History: owens-10276299

CPU User: N/A | Walltime Accuracy: 0.133 | CPU User Balance: N/A | Memory Headroom: N/A

Metric Missing: Unknown Reason

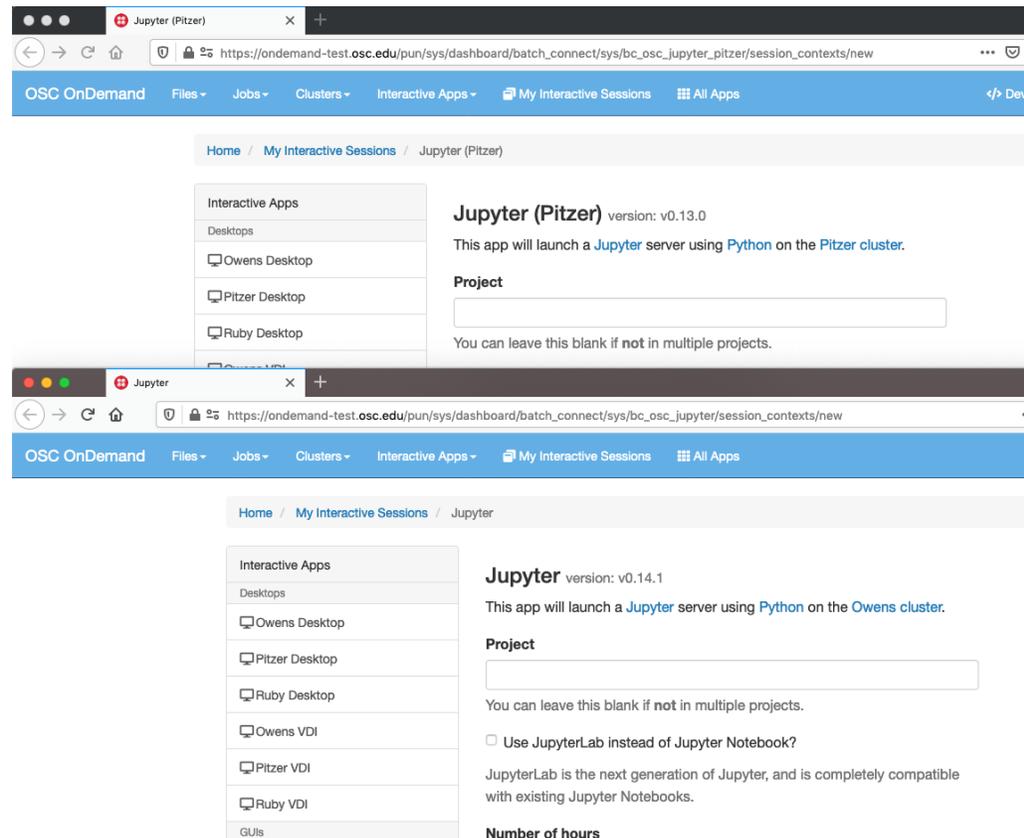
Accounting data | Job script | Executable information | Peers

Key	Value
Category: Administration (11 Items)	
Local Job Id	PZS0714
Organization	Ohio Supercomputer Center
Resource	Owens
Hierarchy Bottom Level	Unknown
PI	PZS0714
PI Institution	Ohio Supercomputer Center
Timezone	US/Eastern
User	efranz
User Institution	Ohio Supercomputer Center
Username	efranz
Category: Allocated resource (6 Items)	
Shared	True
Cores	1
Nodes	1
Total Cores Available	0
Cpu Time	8 seconds
Node Time	8 seconds
Category: Executable (5 Items)	
Name	ondemand/sys/myjobs/basic_sequential
Application	NA
Executable	NA
Exit Status	0
Working directory	NA
Category: Requested resource (3 Items)	
Requested Nodes	1
Requested Wall Time	1 minute
Queue	serial

Accounting data: Shows information about the job that was obtained from the resource manager. This includes timing information such as the start and end time of the job as well as administrative information such as the user that submitted the job and the account that was charged.

1.8 Release: App submit to multiple clusters

Before, one app per cluster:



The screenshot shows the OSC OnDemand web interface. The top navigation bar includes 'OSC OnDemand', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', 'My Interactive Sessions', and 'All Apps'. The main content area shows the configuration for a Jupyter app named 'Jupyter (Pitzer)'. The version is v0.13.0. The description states: 'This app will launch a Jupyter server using Python on the Pitzer cluster.' The 'Project' field is empty. A note says: 'You can leave this blank if not in multiple projects.' The left sidebar shows a list of desktops: Owens Desktop, Pitzer Desktop, and Ruby Desktop.

After, 1 app with cluster dropdown:

Jupyter version: v0.14.1-11-g0db5f85

This app will launch a **Jupyter** server using **Python** on the **Owens cluster**.

Cluster

owens

Project

You can leave this blank if **not** in multiple projects.

Use JupyterLab instead of Jupyter Notebook?

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

Number of hours

1

1.8 Release: Retain completed jobs panel for debugging

The screenshot displays the OnDemand web interface. The top navigation bar includes links for 'Interactive Apps', 'My Interactive Sessions', 'All Apps', 'Develop', 'Help', 'Logged in as efranz', and 'Log Out'. The main content area shows a 'Completed' Jupyter session card for '11044660.owens-batch.ten.osc.edu'. The card details include the creation time '2020-08-24 16:40:31 EDT' and the session ID '3c64256a-90c0-4ab4-be02-72b2a64d1c0f'. A red arrow points from the session ID to a file browser window on the right. The file browser shows a directory listing for '/users/PZS0562/efranz/ondem...' with files such as 'assets', 'share', 'after.sh', 'before.sh', 'config.py', 'connection.yml', 'job_script_content.sh', 'job_script_options.json', 'launch_wrapper.sh', 'output.log', 'script.sh', and 'user_defined_context.json'.

1.8 Release: Dynamic information in job panel via info.html.erb or info.md.erb

MATLAB (11043715.owens-batch.ten.osc.edu) 1 node | 28 cores | Running

Host: >_o0684.ten.osc.edu Delete

Created at: 2020-08-24 12:18:41 EDT

Time Remaining: 30 minutes

Session ID: 38313136-0d8f-4d58-b108-97f0a3a8ff85

For more information see

- [MATLAB Homepage](#)
- [Parallel Computing Toolbox](#)

If you need any help please contact [MATLAB support](#)

noVNC Connection Native Instructions

Compression Image Quality

0 (low) to 9 (high) 0 (low) to 9 (high)

Launch MATLAB View Only (Share-able Link)

RStudio Server (11044697.owens-batch.ten.osc.edu) 1 node | 28 cores | Running

Host: >_o0098.ten.osc.edu Delete

Created at: 2020-08-24 16:53:41 EDT

Time Remaining: 51 minutes

Session ID: e20114de-9019-4617-9800-b728124ef025

As of 2020-08-24 17:02:38 -0400 this job has used 3.9 core hours.
At \$100 per core hour, this job has cost you \$13.92 so far!

Connect to RStudio Server

1.8 patch release

- Fix any issues with OOD-XDMoD integration observed after having a chance to run it in production at OSC
- Address bug fixes that didn't make it into 1.8 release
- Timing – sometime in September

2.0 update

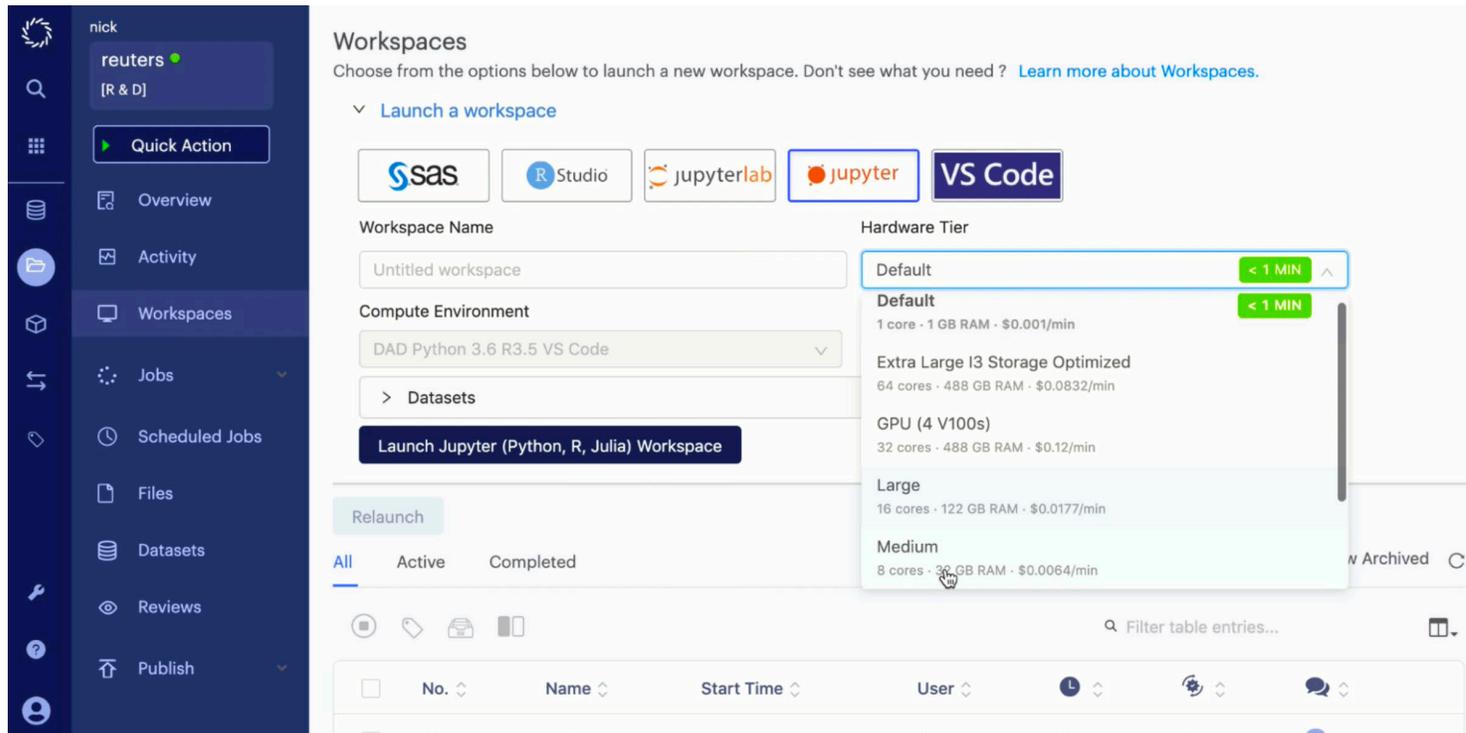
- Timing:
 - Dec 2020
- Interface redesign questions
- Files app questions



Interface redesign

- Looking at two competing designs
 - Telescoping web style interface (add more layers to current)
 - IDE style

Telescoping web page style



- black task bar far left
- purple/blue nav is - could make this list of actions context specific
- left most dark icon folder is selected - so the larger menu is context specific to that files icon; so apps could be
- app as "quick app" appears far most left icon
- low information density
- apps in own pages (what we have now) **but highly customizable**

IDE style

Files

File Edit View Run Kernel Tabs Settings Help

data

Name	Last Modified
1024px-Hubble_Intera...	5 months ago
bar.vl.json	9 minutes ago
Dockerfile	5 months ago
iris.csv	6 months ago
japan_meterological_a...	5 months ago
Museums_in_DC.geoj...	6 months ago
README.md	5 months ago
zika_assembled_gen...	5 months ago

Open a CSV file using Pandas

```
In [5]: 1 import pandas
2 df = pandas.read_csv('../data/iris.csv')
3 df.head(20)
```

```
Out[5]:
```

	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	se
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa
5	5.4	3.9	1.7	0.4	setosa
6	4.6	3.4	1.4	0.3	setosa
7	5.0	3.4	1.5	0.2	setosa
8	4.4	2.9	1.4	0.2	setosa
9	4.9	3.1	1.5	0.1	setosa
10	5.4	3.7	1.5	0.2	setosa
11	4.8	3.4	1.6	0.2	setosa
12	4.8	3.0	1.4	0.1	setosa
13	4.3	3.0	1.1	0.1	setosa
14	5.8	4.0	1.2	0.2	setosa

JupyterLab Demo

JupyterLab: The next generation user interface for Project Jupyter

<https://github.com/jupyter/jupyterlab>

It has been a collaboration between:

- Project Jupyter
- Bloomberg
- Anaconda

1) Building blocks of interactive computing

bar.vl.json 1024px-Hubble

- sites always want their message of the day to show up
- sites want to pin things
- so giving user flexibility to customize their experience is what we are after; but if we take this IDE approach admins are using
- notable features
 - **multiple things open at once**
 - high information density

Files app update

- **Feature parity with the existing app + some basic enhancements (sorting columns, see the owner of the file)**
- Third party storage integration (possibly facilitated with **rclone** or **rclone** is basis for **the files app**)
- Options - order of importance?
 - Cloud drives (Google Drive, 1drive, Box, Dropbox...)
 - Canvas
 - Globus
- Questions:
 - Order of integration
 - Missing?
 - What types of interactions for remotes matter?
 - Viewing/initiating transfers?
 - Batch job wants to interact with remote files
 - File transfer may need job facilitation

2.0 - Other features: Head to Trello

<https://trello.com/b/ksr1g141/open-ondemand-ideas-and-dev>

Other topics?

OPEN  **OnDemand**