

# **HPC at CCR, and Intro to OnDemand**

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# Welcome to Center for Computational Research (CCR)



We are an academic research  
computing center at

University at Buffalo,

State University of New York (SUNY),

Buffalo, New York, USA.

# High-Performance Computing (HPC) at CCR



- CCR houses about 1600 computing **nodes**
- each node has up to 40 processing **cores** (CPUs)
- some have Graphics Processing Units (GPUs)

In total, CCR has about 30,000 CPUs (cores).

# What makes HPC, HPC?

Overall high performance computing features:

- Fast compute
- Data storage
- Substantial memory
- Fast networking
- Specialized software

# Fast compute

CCR has more than 1 PFlop/second peak performance compute capacity

petaflop/s = one quadrillion floating-point operations per second

- processor density (up to 40 cores/node)
- lots of memory (up to 800 GB/node)
- specialized hardware (think GPUs)
- specialized architectures (tuned to scientific problems)

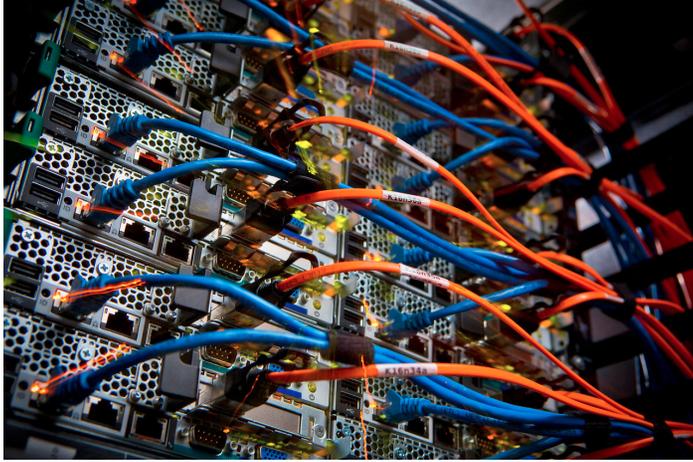
# Lots of data storage



3+ PB high-performance parallel filesystem

(recall: 1 PB =  $2^{50}$  bytes = 1024 terabytes = one million gigabytes)

# High performance networks



- fast connections to data storage
- fast interconnects between compute nodes

# About SLURM



(Yes, the name is a Futurama reference!)

SLURM (*Simple Linux Utility for Resource Management*) is batch scheduling software. It's the gatekeeper on the CCR computing resource.

You tell it about your job's requirements:

- how many *cores*?
- how much *memory*?
- for what *duration*?

# About SLURM II



(Yes, the name is a Futurama reference!)

We must also tell SLURM where to run our job:

- under whose *account*?
- on which *cluster*?
- on which *partition*?

And SLURM schedules your job.

# CCR has three computing clusters:

- general-compute
- industry
- **faculty** (that's us!)

# Faculty cluster

On the faculty cluster, we will use the valhalla partition and these parameters:

```
cluster=faculty  
account=cyberwksp21  
partition=valhalla  
qos=valhalla
```

See for yourself! On the command line, type: `slimits`

# Different ways to run

We can tell SLURM to run:

- `sbatch`:  
schedule a “batch” job when possible
- `salloc/srun`:  
schedule the resources with `salloc`, run interactively with `srun`

**See `salloc` and `srun` in action:**

[salloc demo](#)

# Monitoring: So, what's cooking on the cluster?

What may I access on the cluster?

```
slimits
```

Show me the faculty cluster status:

```
sqstat --faculty
```

Show me valhalla's allocated nodes:

```
snodes all faculty/valhalla | grep alloc
```

output:

```
jsperhac@srv-p22-13:~$ snodes all faculty/valhalla | grep alloc
cpn-f11-03 alloc 24 2:12:1 24/0/0/24 1.00 256000 (null) valhalla FACULT
Y,CPU-E5-2650v4,INTEL
cpn-f11-04 alloc 24 2:12:1 24/0/0/24 1.01 256000 (null) valhalla FACULT
Y,CPU-E5-2650v4,INTEL
cpn-f11-06 alloc 24 2:12:1 24/0/0/24 1.01 256000 (null) valhalla FACULT
Y,CPU-E5-2650v4,INTEL
cpn-f11-07 alloc 24 2:12:1 24/0/0/24 1.01 256000 (null) valhalla FACULT
Y,CPU-E5-2650v4,INTEL
cpn-f11-08 alloc 24 2:12:1 24/0/0/24 1.01 256000 (null) valhalla FACULT
Y,CPU-E5-2650v4,INTEL
cpn-f11-09 alloc 24 2:12:1 24/0/0/24 1.01 256000 (null) valhalla FACULT
Y,CPU-E5-2650v4,INTEL
cpn-f11-10 alloc 24 2:12:1 24/0/0/24 1.01 256000 (null) valhalla FACULT
Y,CPU-E5-2650v4,INTEL
cpn-f11-11 alloc 24 2:12:1 24/0/0/24 1.01 256000 (null) valhalla FACULT
Y,CPU-E5-2650v4,INTEL
cpn-f11-12 alloc 24 2:12:1 24/0/0/24 1.01 256000 (null) valhalla FACULT
Y,CPU-E5-2650v4,INTEL
cpn-p27-15 alloc 12 2:6:1 12/0/0/12 12.01 128000 (null) valhalla FACULT
Y,CPU-E5-2620v3,INTEL
```

# About OnDemand at CCR

During the workshop, we will use a web browser and OnDemand to access CCR computing resources. In some cases the negotiation with SLURM happens behind the scenes.

<https://ondemand.ccr.buffalo.edu>

We will use OnDemand three ways:

- *Jupyter Notebooks*  
notebooks run on a valhalla compute node
- *Faculty Cluster App*  
command line access to a valhalla compute node
- *Faculty Shell*  
command line access to CCR front-end node, vortex



# OnDemand at CCR

This is where we begin: <https://ondemand.ccr.buffalo.edu>

The screenshot shows the CCR OnDemand dashboard in a web browser. The browser's address bar displays the URL <https://ondemand.ccr.buffalo.edu>. The dashboard features a blue navigation bar with the following menu items: CCR OnDemand, Apps, Clusters, Files, Interactive Apps, and Jobs. A red alert banner at the top states: "ALERT: We are aware of issues editing some types of files in the Files app. Please use caution and [view this article for more info](#). See additional announcements in the Message of the Day below." Below the alert is the University at Buffalo logo and the text "Center for Computational Research". A descriptive sentence reads: "OnDemand provides an integrated, single access point for all of your HPC resources." The "Pinned Apps" section includes three tiles: "Active Jobs" (System Installed App), "Home Directory" (System Installed App), and "Academic Cluster Shell Access" (System Installed App). To the right, two efficiency reports are displayed. The "Jobs Efficiency Report - 2021-05-11 to 2021-06-10" shows 85.4% efficient and 14.6% inefficient jobs, with a bar chart and the text "146 inefficient jobs / 999 total jobs". The "Core Hours Efficiency Report - 2021-05-11 to 2021-06-10" shows 99.6% efficient and 0.4% inefficient core hours, with a bar chart and the text "5.1 inefficient core hours / 1249.4 total core hours". At the bottom, a "Desktops" section shows four monitor icons representing different clusters: Academic Cluster (UB-...), Academic Cluster (UB-...), Faculty Cluster, and Faculty Cluster.



# OnDemand Jupyter Notebooks

Schedule a SLURM job that runs a Jupyter session on a valhalla compute node:

[Interactive Apps -> Jupyter Notebook Quantum Chemistry](#)

1. Start the  
Interactive  
App:

Dashboard - CCR OnDemand

https://ondemand.ccr.buffalo.edu

CCR OnDemand Apps Clusters Files Interactive Apps Jobs

**NEW USERS:** Run this script in the terminal before running...  
**MACHINE STATUS:** Academic cluster status, Industry...  
**NEXT DOWNTIME:** Tuesday, June 29, 2021 More details...  
**VIRTUAL WORKSHOPS:** Check out our library of virtual...  
**FOLLOW US!** CCR is on Twitter - Get system status updates...  
**IMPORTANT ACCOUNT POLICY CHANGE** Coming 7/2... accounts. SSH logins will no longer accept passwords...

**University at Buffalo**  
**Center for Computational Research**

OnDemand provides an integrated, single access point for all your computing needs.

**Pinned Apps** A featured subset of all available apps.

- Active Jobs
- Home Directory
- Academic Cluster Shell Access

System Installed App

**Interactive Apps**

- Desktops
  - Academic Cluster (UB-HPC) Desktop
  - Academic Cluster (UB-HPC) Desktop - Advanced Options
  - Faculty Cluster Desktop
  - Faculty Cluster Desktop - Advanced Options
  - Viz Node - CUDA Desktop
  - Viz Node - OpenGL Desktop
  - Viz Node - OpenGL DISABLED Desktop
- GUIs
  - MATLAB
- Notebooks
  - Jupyter Notebook - Academic Cluster
  - Jupyter Notebook - Faculty Cluster
  - Jupyter Notebook Quantum Chemistry
- Web Portals
  - Coldfront
  - Helpdesk & Searchable Knowledgebase
  - WebMO
  - XDMoD Job Statistics

into Open XDMoD first, and then try again.

https://ondemand.ccr.buffalo.edu/pun/sys/dashboard/batch\_connect/sys/jupyter\_quantum\_chem/session\_contexts/new

# OnDemand Jupyter Notebooks

Schedule a SLURM job that runs a Jupyter session on a valhalla compute node:

Interactive Apps -> Jupyter Notebook Quantum Chemistry

2. Configure the session  
(Specify SLURM parameters):

## Interactive Apps

## Desktops

Academic Cluster (UB-HPC) Desktop

Academic Cluster (UB-HPC) Desktop - Advanced Options

Faculty Cluster Desktop

Faculty Cluster Desktop - Advanced Options

Viz Node - CUDA Desktop

Viz Node - OpenGL Desktop

Viz Node - OpenGL DISABLED Desktop

## GUIs

MATLAB

## Notebooks

Jupyter Notebook - Academic Cluster

Jupyter Notebook - Faculty Cluster

Jupyter Notebook Quantum Chemistry

## Jupyter Notebook Quantum Chemistry

This app will launch a Jupyter notebook on the Valhalla partition of the faculty cluster. You must have access to this cluster or your job will not run. The longest allowable wall time for these nodes is 30 days. It is recommended that you enter only the time you need to run your job rather than use the default.

## Account

## Number of hours

## Number of nodes

## Number of Cores

## Number of cores per node

## Node Features

Enter feature(s), separated by commas, for node types you want to access including high speed networks, CPU and GPU types. Use the command 'snodes all faculty/valhalla' in a terminal window to see available features

## Amount of Memory Per Node

Enter the amount of memory you want to request, per node, in megabytes (MB).

Exclude host



# OnDemand Jupyter Notebooks

Schedule a SLURM job that runs a Jupyter session on a valhalla compute node:

[Interactive Apps -> Jupyter Notebook Quantum Chemistry](#)

3. Run Jupyter:

<input type="checkbox"/>	folder	jupyter-kernel-example	23 days ago	
<input type="checkbox"/>	folder	largemem	5 years ago	
<input type="checkbox"/>	folder	ondemand	2 years ago	
<input type="checkbox"/>	folder	R-scripts	4 years ago	
<input type="checkbox"/>	folder	renderbot-test	7 years ago	
<input type="checkbox"/>	folder	rlibs	3 years ago	
<input type="checkbox"/>	folder	simple-jobarray	a year ago	
<input type="checkbox"/>	folder	snowfall	3 years ago	
<input type="checkbox"/>	folder	submit-test-success-debug-8512468	3 years ago	
<input type="checkbox"/>	folder	submit-tests	4 months ago	
<input type="checkbox"/>	folder	test	4 months ago	
<input type="checkbox"/>	folder	test-eman2-mpi	4 years ago	
<input type="checkbox"/>	folder	UB-Box	8 months ago	
<input type="checkbox"/>	folder	workshop	9 days ago	
<input type="checkbox"/>	file	check-libra-plus-pkgs.ipynb	14 days ago	1.36 kB
<input type="checkbox"/>	file	test-qmflows-pkgs.ipynb	Running 14 days ago	1.21 kB
<input type="checkbox"/>	file	Untitled.ipynb	9 days ago	1.05 kB
<input type="checkbox"/>	file	Untitled1.ipynb	7 days ago	2.92 kB
<input type="checkbox"/>	file	ergoscf.out	a year ago	5.65 kB
<input type="checkbox"/>	file	input_tmp.in	8 days ago	0 B
<input type="checkbox"/>	file	job-8528567.tar.gz	3 years ago	426 B
<input type="checkbox"/>	file	junk-activate-libra-env.sh	3 months ago	430 B
<input type="checkbox"/>	file	monitorSLURM.py	a year ago	21.4 kB
<input type="checkbox"/>	file	Rplots.pdf	3 years ago	3.61 kB
<input type="checkbox"/>	file	this-file.txt	a day ago	93 B
<input type="checkbox"/>	file	trythis.txt	a day ago	38 B
<input type="checkbox"/>	file	yum-list-installed.txt	3 years ago	86.1 kB



# OnDemand Faculty Cluster App

Schedule a SLURM job that runs a Linux desktop on a valhalla compute node:

[Interactive Apps -> Faculty Cluster Desktop - Advanced Options](#)

*Share the cores!*

1. Start the  
Interactive  
App:

My Interactive Sessions - [X] +

https://ondemand.ccr.buffalo.edu 90% Search

CCR OnDemand Apps Clusters Files Interactive Apps Jobs

**ALERT:** We are aware of issues editing some types of [truncated] for more info See additional announcements in the Message of the [truncated]

Session was successfully created.

Home / My Interactive Sessions

**Interactive Apps**

- Desktops
  - Academic Cluster (UB-HPC) Desktop
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  - Faculty Cluster Desktop - Advanced Options
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  - Coldfront
  - Helpdesk & Searchable Knowledgebase
  - WebMO
  - XDMoD Job Statistics

**Jupyter Notebook**

Host: >\_cpn-p27-17

Created at: 2021-06-10

Time Remaining: 3 h

Session ID: bbad5296

Connect to Jupyter

**Faculty Cluster Desktop**

Created at: 2021-06-09 10:20:23 EDT

Session ID: c5976488-131a-442f-b66a-012a81a41398

Delete

For debugging purposes, this card will be retained for 6 more days

https://ondemand.ccr.buffalo.edu/pun/sys/dashboard/ba...ct/sys/bc\_desktop/21-faculty\_adv/session\_contexts/new



# OnDemand Faculty Cluster App

Schedule a SLURM job that runs a Linux desktop on a valhalla compute node:

[Interactive Apps -> Faculty Cluster Desktop - Advanced Options](#)

*Share the cores!*

2. Specify  
SLURM  
parameters:

## Interactive Apps

## Desktops

Academic Cluster (UB-HPC) Desktop

Academic Cluster (UB-HPC) Desktop - Advanced Options

Faculty Cluster Desktop

Faculty Cluster Desktop - Advanced Options

Viz Node - CUDA Desktop

Viz Node - OpenGL Desktop

Viz Node - OpenGL DISABLED Desktop

## GUIs

MATLAB

## Notebooks

Jupyter Notebook - Academic Cluster

Jupyter Notebook - Faculty Cluster

Jupyter Notebook

## Faculty Cluster Desktop - Advanced Options

This app will launch an interactive desktop on one or more compute nodes in the faculty cluster. You must have access to this cluster or your job will not run. The longest allowable wall time for these nodes varies from 72 hours to 30 days depending on the partition. It is recommended that you enter only the time you need to run your job rather than use the default.

### Slurm Account

Leave blank unless you have access to more than one

### Partition

Please select a partition from the drop-down menu

### QOS

Enter the same as the partition name

### Number of hours

### Number of nodes

### Number of Cores

Number of cores per node

### Node Features



# OnDemand Faculty Cluster App

Schedule a SLURM job that runs a Linux desktop on a valhalla compute node:

[Interactive Apps -> Faculty Cluster Desktop - Advanced Options](#)

*Share the cores!*

3. Run Cluster  
Desktop:



jsperhac@cpn-p27-16: ~

File Edit View Search Terminal Help

jsperhac@cpn-p27-16:~\$





# OnDemand Faculty Shell

Run a command line shell on CCR's front-end node, vortex:

[Clusters -> Faculty Cluster Shell Access](#)

Note: It's not a running job, just a shell. Use the shell to run a SLURM script, or a modest test (few minutes' duration, low memory requirements).

# 1. Start the shell:

The screenshot shows the CCR OnDemand web interface. The 'Interactive Apps' dropdown menu is open, displaying various desktop and notebook options. The 'Faculty Cluster Desktop - Advanced Options' option is highlighted. The interface also shows a navigation bar with 'My Interactive Sessions' and a sidebar with 'Interactive Apps' and 'Jupyter Notebook' sections.

- Desktops
  - Academic Cluster (UB-HPC) Desktop
  - Academic Cluster (UB-HPC) Desktop - Advanced Options
  - Faculty Cluster Desktop
  - Faculty Cluster Desktop - Advanced Options
  - Viz Node - CUDA Desktop
  - Viz Node - OpenGL Desktop
  - Viz Node - OpenGL DISABLED Desktop
- GUIs
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  - Jupyter Notebook - Academic Cluster
  - Jupyter Notebook - Faculty Cluster
  - Jupyter Notebook Quantum Chemistry
- Web Portals
  - Coldfront
  - Helpdesk & Searchable Knowledgebase
  - WebMO
  - XDMoD Job Statistics

URL: [https://ondemand.ccr.buffalo.edu/pun/sys/dashboard/ba...ct/sys/bc\\_desktop/21-faculty\\_adv/session\\_contexts/new](https://ondemand.ccr.buffalo.edu/pun/sys/dashboard/ba...ct/sys/bc_desktop/21-faculty_adv/session_contexts/new)

# 2. Run the shell:

The screenshot shows a terminal window with the shell prompt `jsperhac@srv-p22-12:~`. The terminal displays system information, including the next downtime, maintenance schedule, and a list of virtual workshops. The prompt is followed by a red cursor.

```
Next Downtime: Tuesday, June 29, 2021
Maintenance Downtime Schedule: https://tinyurl.com/downtime-schedule

#####

Questions or Problems? Check out our searchable knowledgebase:
https://ubccr.freshdesk.com

#####

Check out our virtual workshops:
https://ubccr.freshdesk.com/en/support/solutions/articles/13000074205-virtual-workshops

#####

New quota usage - you must specify path:
iquota -p /user/username
iquota -p /projects/academic/yourgroup
iquota -p /panasas/scratch/grp-yourgroup

More details: https://ubccr.freshdesk.com/support/solutions/articles/5000684891

#####

IMPORTANT: ACCOUNT POLICY CHANGE COMING 7/27/21
Two factor authentication will be required on all CCR accounts. SSH logins will no longer
accept passwords; SSH keys must be used. More details: https://tinyurl.com/2fapolicy

#####

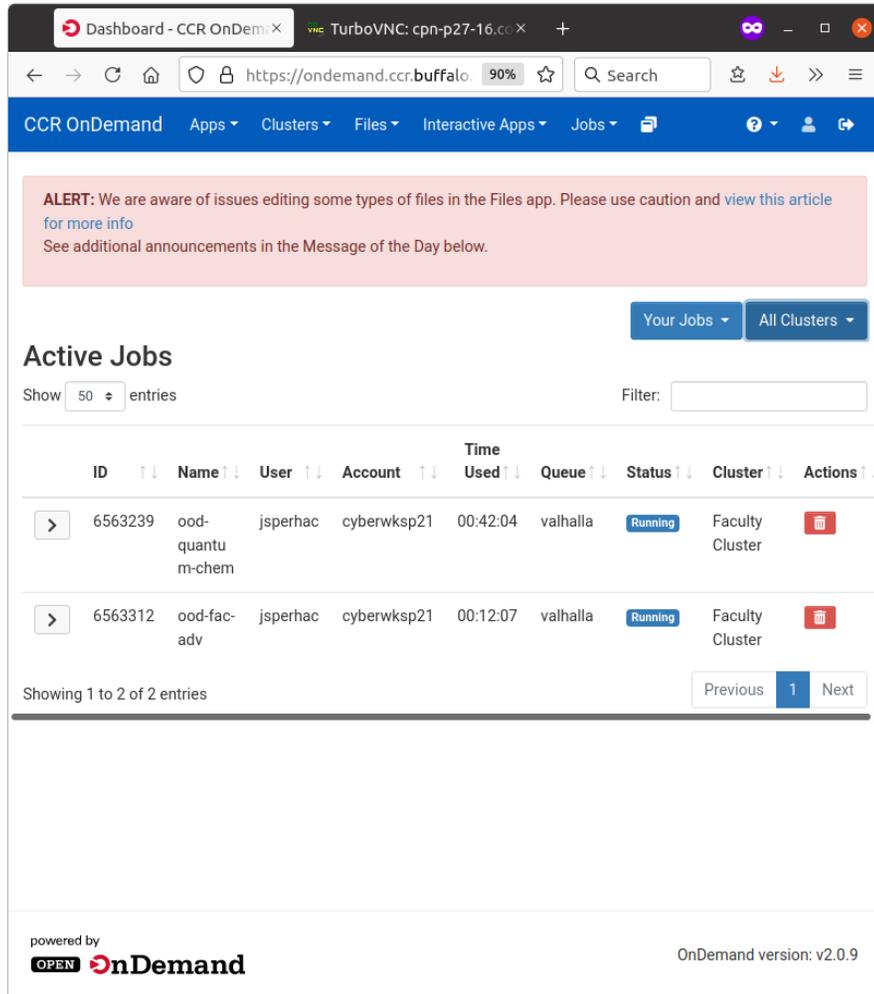
jsperhac@srv-p22-12:~$
```

# View your active jobs

View jobs you are running right now:

[Jobs -> Active Jobs](#)

# 1. View in OnDemand:



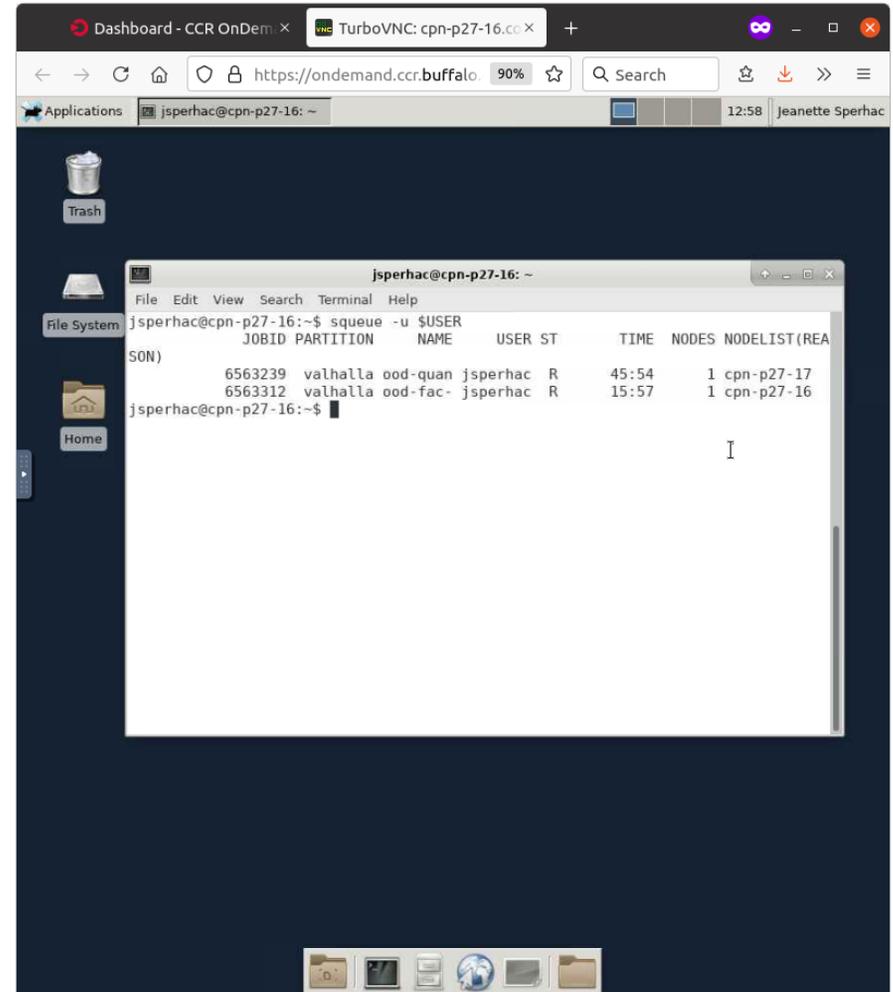
The screenshot shows the OnDemand web interface. At the top, there is a navigation bar with "CCR OnDemand" and various menu items. Below the navigation bar, there is an alert message: "ALERT: We are aware of issues editing some types of files in the Files app. Please use caution and view this article for more info. See additional announcements in the Message of the Day below." The main content area is titled "Active Jobs" and features a table with columns for ID, Name, User, Account, Time Used, Queue, Status, Cluster, and Actions. Two jobs are listed: one with ID 6563239 and another with ID 6563312. The interface also includes a search bar, a filter input, and pagination controls.

ID	Name	User	Account	Time Used	Queue	Status	Cluster	Actions
6563239	ood-quantu m-chem	jsperhac	cyberwksp21	00:42:04	valhalla	Running	Faculty Cluster	
6563312	ood-fac-adv	jsperhac	cyberwksp21	00:12:07	valhalla	Running	Faculty Cluster	

Showing 1 to 2 of 2 entries

powered by **OPEN OnDemand** OnDemand version: v2.0.9

# 2. Or run `queue -u $USER` in a terminal:



The screenshot shows a terminal window on a Linux system. The terminal prompt is `jsperhac@cpn-p27-16:~$`. The command `queue -u $USER` has been executed, resulting in the following output:

```
jsperhac@cpn-p27-16:~$ queue -u $USER
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
6563239 valhalla ood-quantu jsperhac R 45:54 1 cpn-p27-17
6563312 valhalla ood-fac-adv jsperhac R 15:57 1 cpn-p27-16
jsperhac@cpn-p27-16:~$
```

# Troubleshoot and debug

View your OnDemand sessions (Click on the box icon, My Interactive Sessions):

My Interactive Sessions - x vnc TurboVNC: cpn-p27-16.cc x

https://ondemand.ccr.buffalo.edu 90% Search

CCR OnDemand Apps Clusters Files Interactive Apps Jobs

**ALERT:** We are aware of issues editing some types of files in the Files app. Please use caution and [view this article for more info](#). See additional announcements in the Message of the Day below.

Home / My Interactive Sessions

**Interactive Apps**

Desktops

- Academic Cluster (UB-HPC) Desktop
- Academic Cluster (UB-HPC) Desktop - Advanced Options
- Faculty Cluster Desktop
- Faculty Cluster Desktop - Advanced Options
- Viz Node - CUDA Desktop
- Viz Node - OpenGL Desktop
- Viz Node - OpenGL DISABLED

**Faculty Cluster Desktop - Advanced Options (6563312)**  
1 node | 4 cores | Running

Host: >\_cpn-p27-16.compute.cbis.ccr.buffalo.edu Delete

Created at: 2021-06-10 12:39:29 EDT

Time Remaining: 37 minutes

Session ID: 7a7b093e-528d-432d-9058-4c1684b63fe6

Compression: 0 (low) to 9 (high) Image Quality: 0 (low) to 9 (high)

Launch Faculty Cluster Desktop - Advanced Options

View Only (Share-able Link)

**Jupyter Notebook Quantum Chemistry (6563239)**  
1 node | 1 core | Running

Host: >\_cpn-p27-17.compute.cbis.ccr.buffalo.edu Delete

https://ondemand.ccr.buffalo.edu/pun/sys/dashboard/batch\_connect/sessions

# Troubleshoot and debug: zoom in on one session

For each session we see useful information:

- Note the hostname where the job is running, cpn-p27-15
- You can click Session ID to access session log files

Faculty Cluster Desktop - Advanced Options (6550282)

1 node | 4 cores | Running

Host: [\\_cpn-p27-15.compute.cbis.ccr.buffalo.edu](https://>_cpn-p27-15.compute.cbis.ccr.buffalo.edu) Delete

Created at: 2021-06-09 08:46:46 EDT

Time Remaining: 59 minutes

Session ID: [007b37de-20d7-42d9-8728-def54a96e726](#)

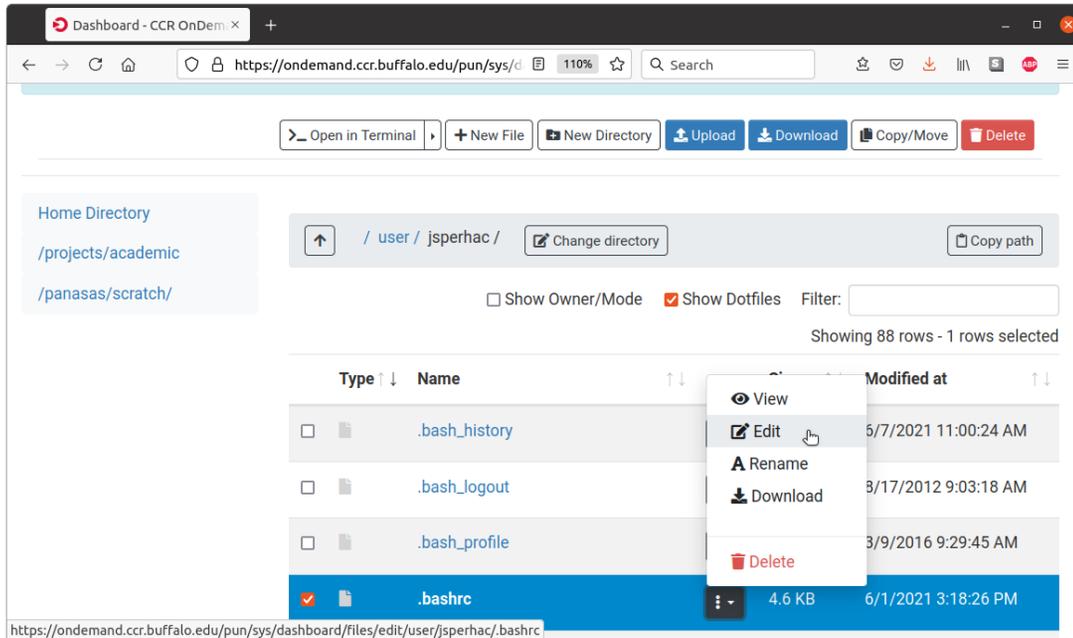
---

Compression Image Quality

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

Launch Faculty Cluster Desktop - Advanced Options View Only (Share-able Link)

# Files app



Use the OnDemand Files app (e.g. Files -> Home Directory) for:

- Browsing directories
- Upload files
- Download files
- Simple file edits\*

\* Potentially

# Editing your files

You have multiple options for file editor:

- OnDemand Files app\* (simplest)
- nano (easy)
- vi (just right)
- emacs (grrr)

\* Potentially

# Contact us

Have a question, comment, or issue?

- Join us on the workshop Slack channel:

[quantumdynamicslab.slack.com](https://quantumdynamicslab.slack.com)

- Check the [CCR documentation](#)

- Enter a CCR help ticket:

email: [ccr-help@buffalo.edu](mailto:ccr-help@buffalo.edu)

webpage: <https://ubccr.freshdesk.com/>