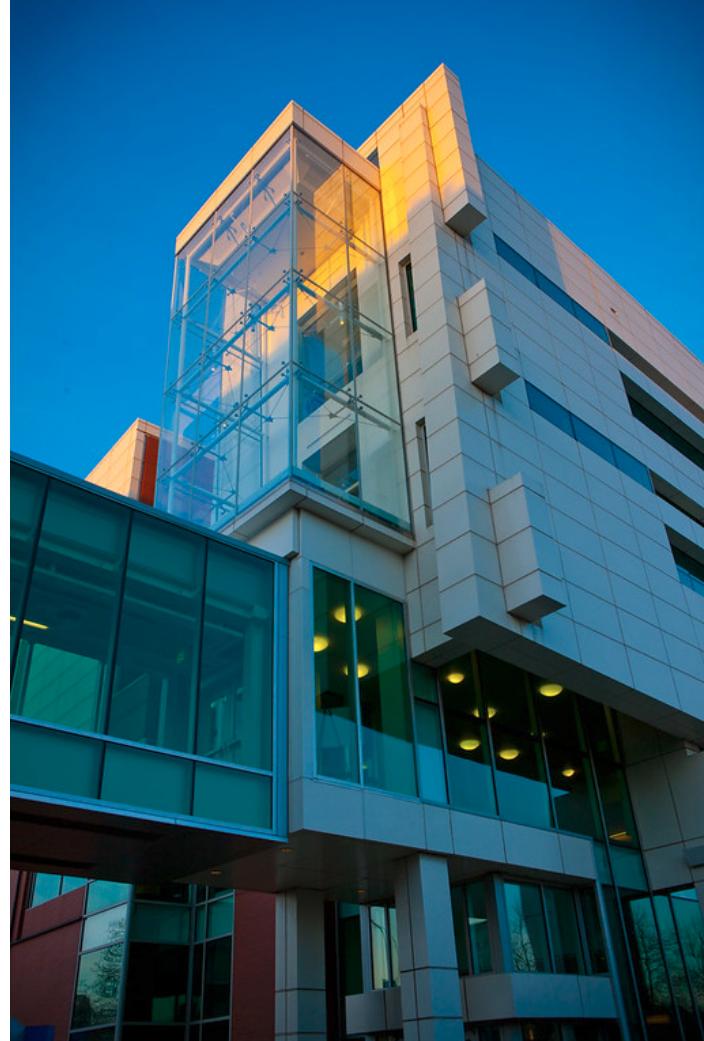


HPC at CCR, and Intro to OnDemand

Jeanette Sperhac

14 June 2021

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)

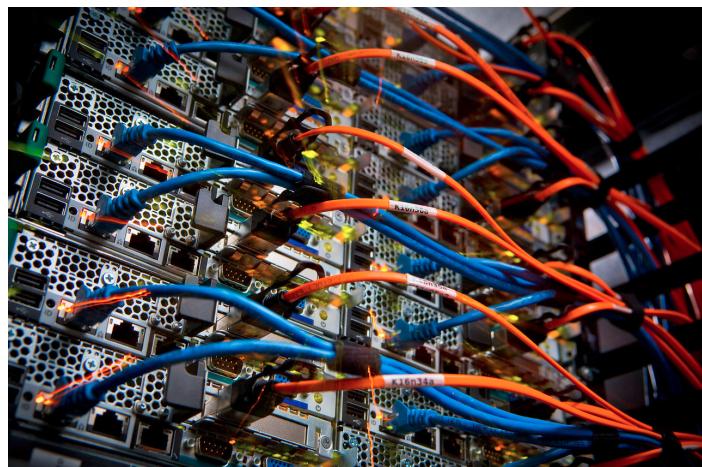
Lots of data storage



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



We must also tell SLURM where to run our job:

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

And SLURM schedules your job.

(Yes, the name
is a Futurama
reference!)

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. At the top, there's a browser header with the URL <https://ondemand.ccr.buffalo.edu>. Below the header is a blue navigation bar with links for "CCR OnDemand", "Apps", "Clusters", "Files", "Interactive Apps", "Jobs", and other user options.

A red alert box in the center-left area contains the text: "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 features the University at Buffalo logo and the Center for Computational Research name. It states: "OnDemand provides an integrated, single access point for all of your HPC resources."

Pinned Apps (A featured subset of all available apps)

- Active Jobs**: System Installed App
- Home Directory**: System Installed App
- Academic Cluster Shell Access**: System Installed App

Jobs Efficiency Open XDMoD Report - 2021-05-11 to 2021-06-10

85.4% efficient 14.6% inefficient

146 inefficient jobs / 999 total jobs

Core Hours Efficiency Open XDMoD Report - 2021-05-11 to 2021-06-10

99.6% efficient 0.4% inefficient

5.1 inefficient core hours / 1249.4 total core hours

Desktops

- Academic Cluster (UB-HPC) Desktop
- Academic Cluster (UB-HPC) Desktop
- Faculty Cluster Desktop
- Faculty Cluster Desktop

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:

VNC noVNC Dashboard - noVNC eastern dayli vhub - Tools: +

https://ondemand.ccr.buffalo.edu/ 110% Search

CCR OnDemand Apps Clusters Files Interactive Apps Jobs ? User Help

NEW USERS: Run this script in the terminal before running your first job.

MACHINE STATUS: Academic cluster status, Industry cluster status

NEXT DOWNTIME: Tuesday, June 29, 2021 [More details](#)

VIRTUAL WORKSHOPS: Check out our library of virtual workshops

FOLLOW US! CCR is on Twitter - [Get system status updates](#)

IMPORTANT ACCOUNT POLICY CHANGE Coming 7/2/2021: Accounts will no longer accept passwordless logins. SSH logins will no longer accept passwords.

University at Buffalo
Center for Computational Research

OnDemand provides an integrated, single access point to all of the University's computing resources.

Pinned Apps A featured subset of [all available applications](#)

- Active Jobs
- Home Directory
- Academic Cluster Shell Access

System Installed App System Installed App System

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

INFO 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):

[←](#) [→](#) [⟳](#) [↑](#) [↓](#) [🔒](#) [🔓](#) https://ondemand.ccr.buffalo.edu/jupyter-notebook/ 90% [☆](#)[🔍 Search](#)

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

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.

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:

[←](#) [→](#) [C](#) [A](#)

https://ondemand.ccr.buffalo.edu

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Search



>>



jupyter

[Quit](#)[Logout](#)

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

[CCR OnDemand](#)[Apps](#)[Clusters](#)[Files](#)[Interactive Apps](#)[Jobs](#)

ALERT: We are aware of issues editing some types of
for more info

See additional announcements in the Message of the Day

Session was successfully created.

[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

Jupyter Notebook

Host: >_cpn-p27-17

Created at: 2021-06-10

Time Remaining: 3 hours

Session ID: bbad5296

Connect to Jupyter

Faculty Cluster Desktop

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

Delete

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

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

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

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:

[←](#) [→](#) [C](#) [A](#)

https://ondemand.ccr.buffalo.edu

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Search



Interactive Apps

Desktops

Academic Cluster
(UB-HPC) DesktopAcademic Cluster
(UB-HPC) Desktop -
Advanced OptionsFaculty Cluster
DesktopFaculty Cluster
Desktop - Advanced
OptionsViz Node - CUDA
DesktopViz Node -
OpenGL DesktopViz Node -
OpenGL DISABLED
Desktop

GUIs

MATLAB

Notebooks

Jupyter Notebook
- Academic ClusterJupyter 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:

My Interactive Sessions -

TurboVNC: cpn-p27-16.co



-

□

×

← → C ⌘ ⌘



https://ondemand.ccr.buffalo.

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Search



>>



Applications

jsperhac@cpn-p27-16: ~



12:41

Jeanette Sperhac



Trash



File System



Home



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. A modal window is open, listing various desktop and Jupyter Notebook options. The 'Faculty Cluster Desktop - Advanced Options' option is highlighted. The main page displays an 'ALERT' message about issues with editing some types of info, a success message about a session being created, and navigation links for Home and My Interactive Sessions. The sidebar on the left lists categories like Desktops, Academic Cluster (UB-HPC) Desktop, and Faculty Cluster Desktop.

ALERT: We are aware of issues editing some types of info
See additional announcements in the Message of the Day

Session was successfully created.

Home / My Interactive Sessions

Interactive Apps

Jupyter Notebook

Host: >cpn-p27-17

Created at: 2021-06-10

Time Remaining: 3 hours

Session ID: bbad5296

Connect to Jupyter

Faculty Cluster Desktop

Faculty Cluster Desktop - Advanced Options

Viz Node - CUDA Desktop

Viz Node - OpenGL Desktop

Desktops

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

- Jupyter Notebook - Academic Cluster
- Jupyter Notebook - Faculty Cluster
- Jupyter Notebook Quantum Chemistry

Web Portals

- Coldfront
- Helpdesk & Searchable Knowledgebase
- WebMO
- XDMoD Job Statistics

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

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

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

2. Run the shell:

The screenshot shows a terminal window with a black background. It displays several system messages and a command prompt. The messages include information about downtime, maintenance, quota usage, account policy changes, and two-factor authentication requirements. The command prompt shows the user's session ID and a red cursor.

Host: voriex.cbls.ccr.buffalo.edu

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/1300074205-virtual-workshops>

#####

New iquota 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/2fpolicy>

#####

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 CCR OnDemand web interface. At the top, there's a banner with 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". Below this, the "Active Jobs" section displays two running jobs:

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

At the bottom, it says "Showing 1 to 2 of 2 entries".

2. Or run squeue -u \$USER in a terminal:

The screenshot shows a terminal window titled "jsperhac@cpn-p27-16: ~". The user has run the command "squeue -u \$USER". The output is as follows:

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(READY)
6563239	valhalla	ood-quantum-chem	jsperhac	R	45:54	1	cpn-p27-17
6563312	valhalla	ood-fac-adv	jsperhac	R	15:57	1	cpn-p27-16

Troubleshoot and debug

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

My Interactive Sessions - X TurboVNC: cpn-p27-16.co 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.cbls.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.cbls.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.cbls.ccr.buffalo.edu Delete

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

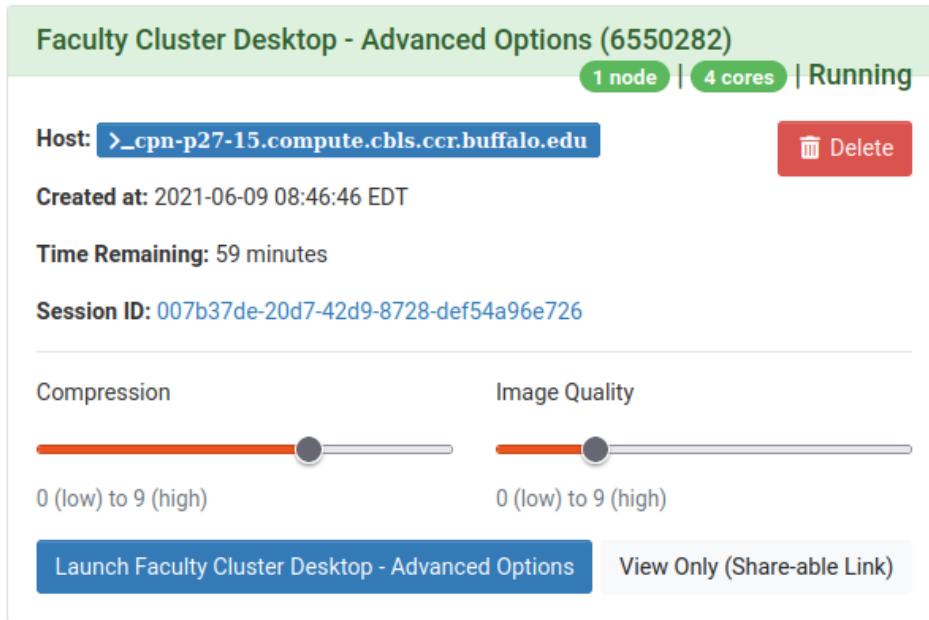
Time Remaining: 59 minutes

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

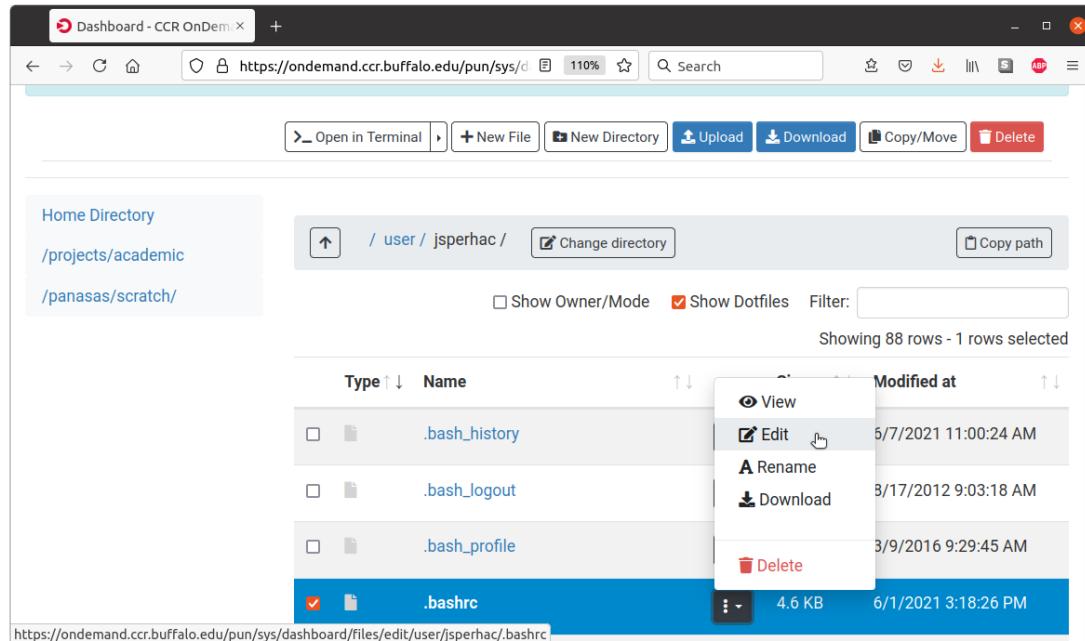
Compression  Image Quality 

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:

quantumdynamicshub.slack.com

- Check the CCR documentation

- Enter a CCR help ticket:

email: ccr-help@buffalo.edu

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