HPC at CCR, and Intro to OnDemand

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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

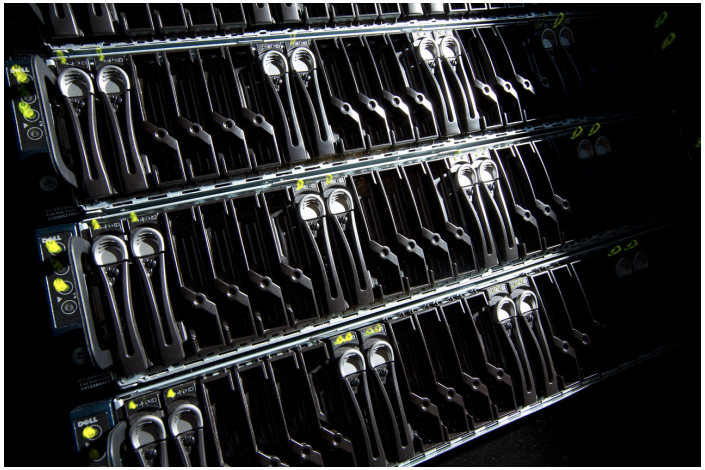
Fast compute

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)

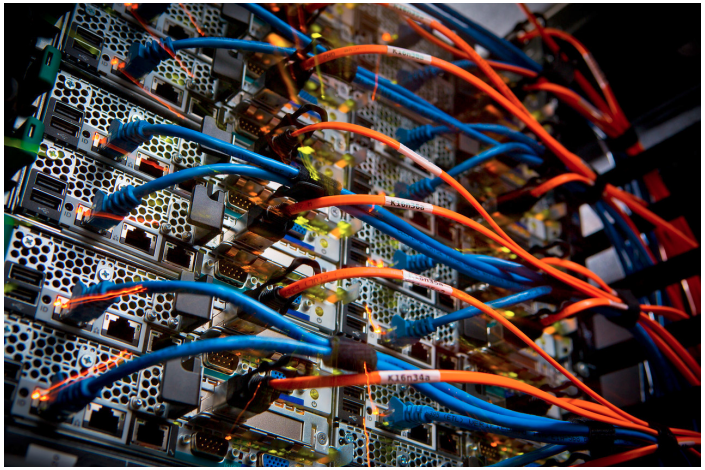
Lots of data storage



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

(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*

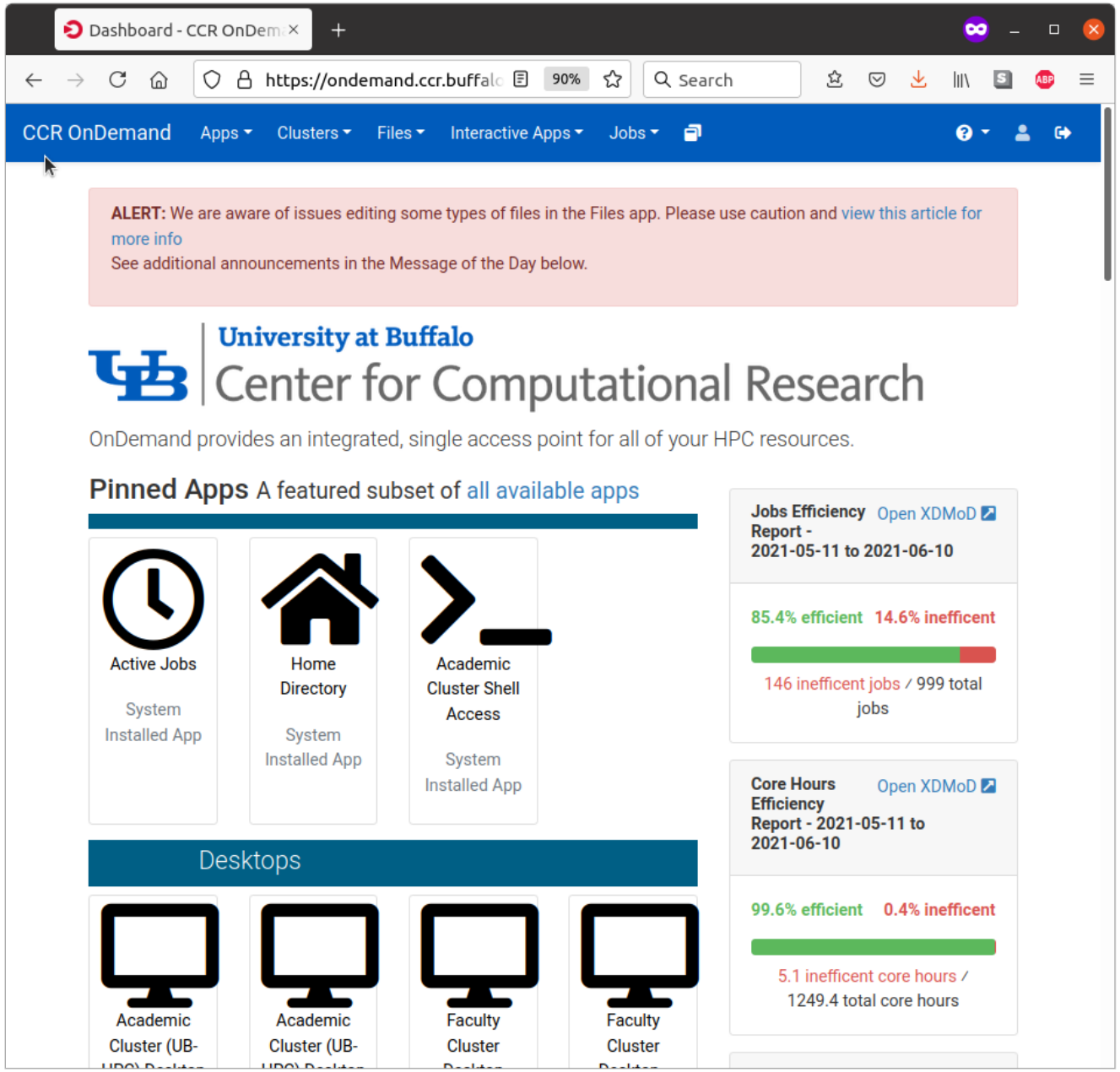
  command line access to a `valhalla` compute node

- *Faculty Shell*

  command line access to CCR front-end node, `vortex`

OnDemand at CCR

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

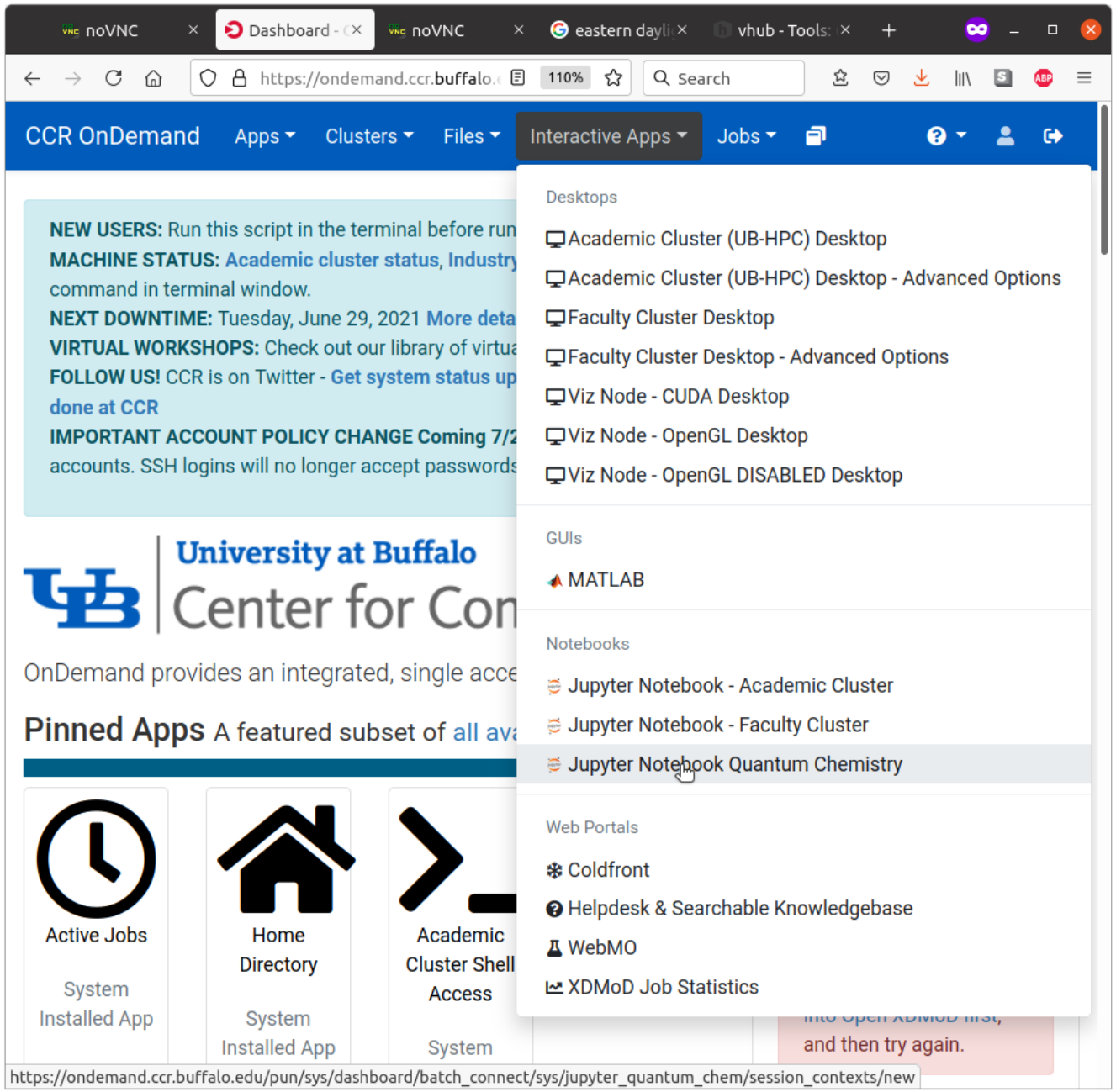


OnDemand Jupyter Notebooks

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:


noVNC
Dashboard -
noVNC
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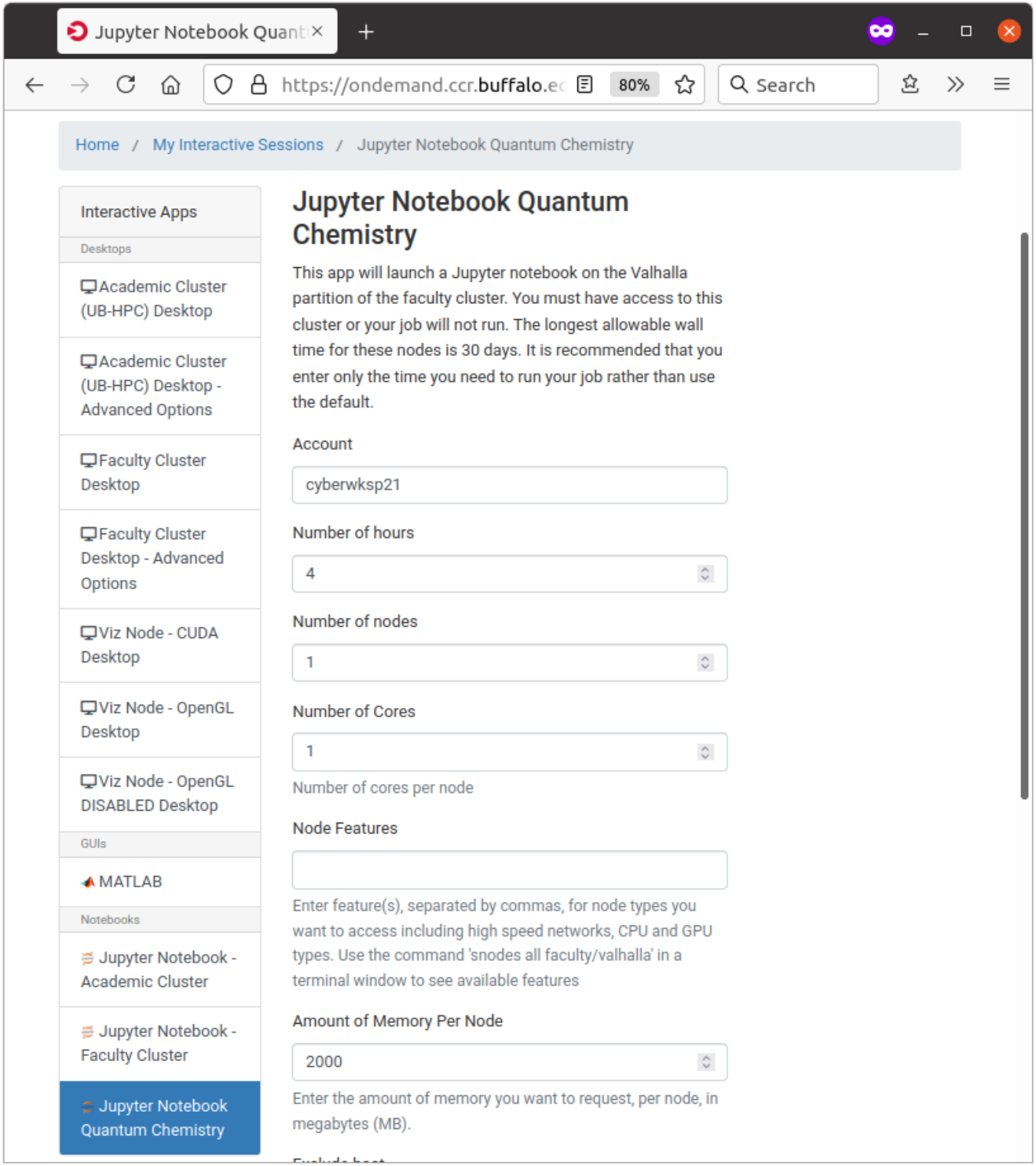
NEW USERS: Run this script in the terminal before run
MACHINE STATUS: Academic cluster status, Industry
command in terminal window.
NEXT DOWNTIME: Tuesday, June 29, 2021 More deta
VIRTUAL WORKSHOPS: Check out our library of virtua
FOLLOW US! CCR is on Twitter - Get system status up
done at CCR
IMPORTANT ACCOUNT POLICY CHANGE Coming 7/2
accounts. SSH logins will no longer accept passwords
University at Buffalo
Center for Con
OnDemand provides an integrated, single acce
Pinned Apps A featured subset of all ava
Active Jobs
System Installed App
Home Directory
System Installed App
Academic Cluster Shell Access
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
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):


Jupyter Notebook Quant
https://ondemand.ccr.buffalo.ec
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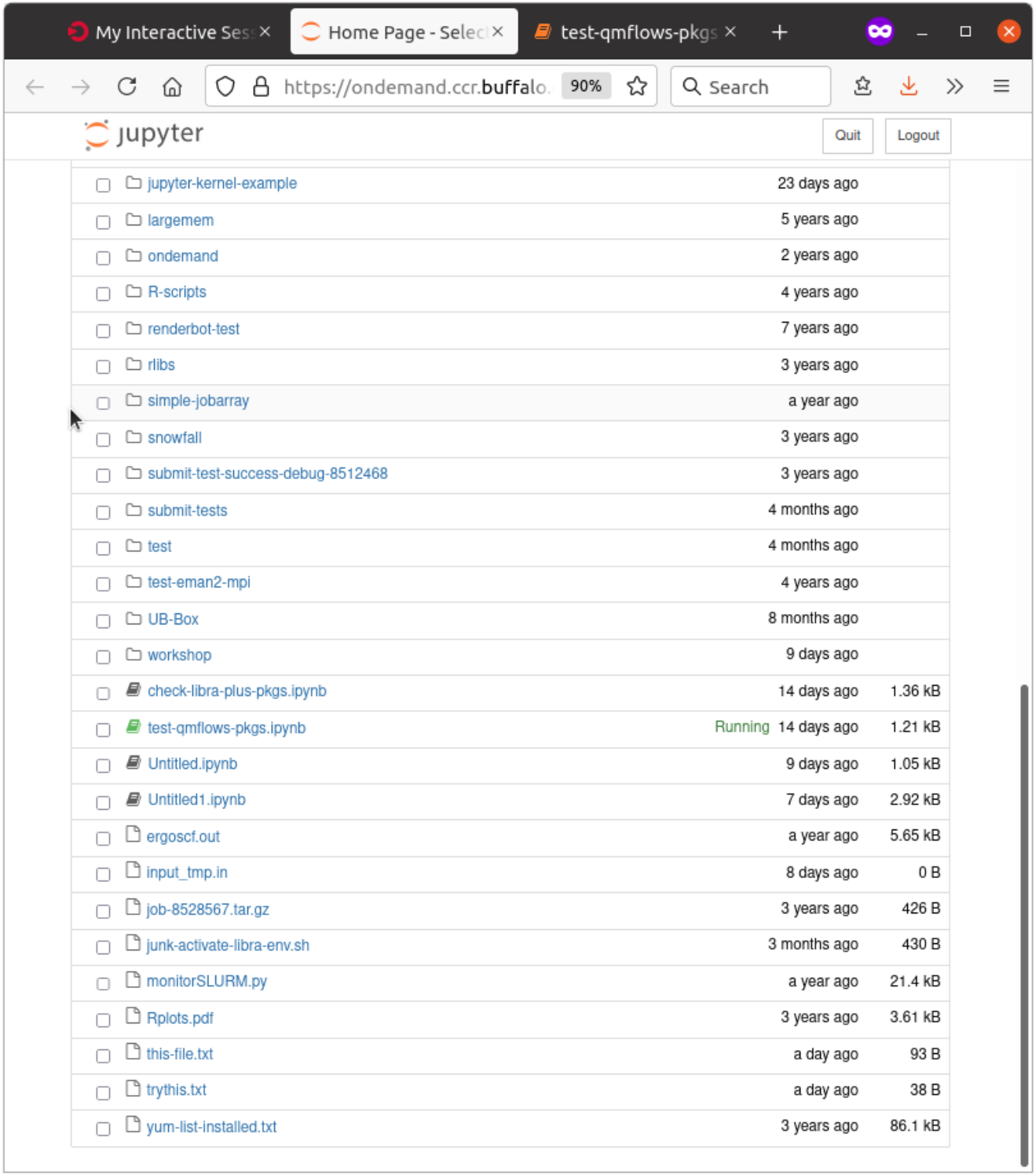
Search
Home / My Interactive Sessions / Jupyter Notebook Quantum Chemistry
Interactive Apps
Desktops
Academic Cluster (UB-HPC) Desktop
Academic Cluster (UB-HPC) Desktop - Advanced Options
Faculty Cluster Desktop
Faculty Cluster Desktop - Advanced Options
Viz Node - CUDA Desktop
Viz Node - OpenGL Desktop
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
cyberwksp21
Number of hours
4
Number of nodes
1
Number of Cores
1
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
2000
Enter the amount of memory you want to request, per node, in megabytes (MB).

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

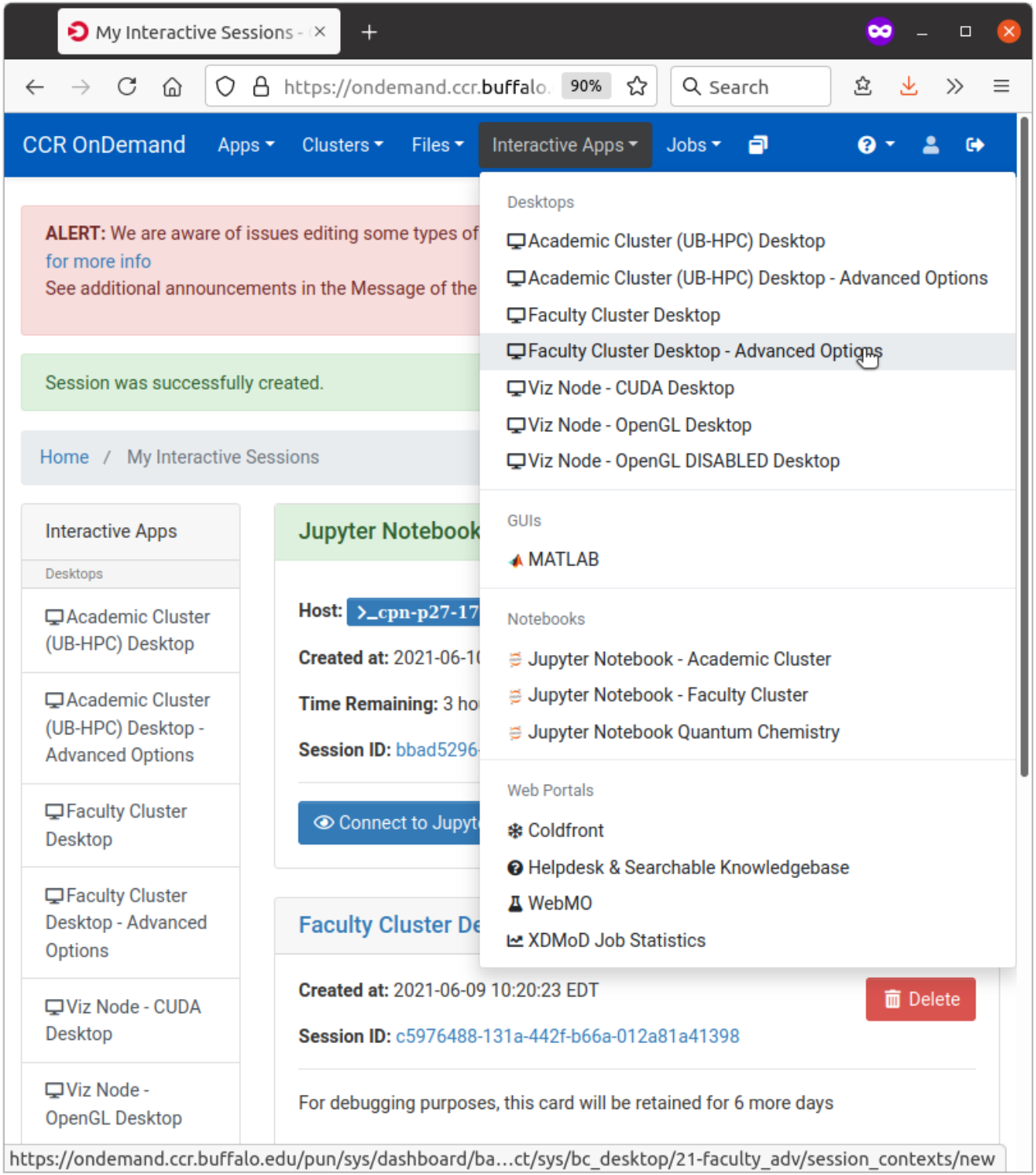
OnDemand Faculty Cluster App

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: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Jupyter Notebook - Faculty Cluster
Jupyter Notebook Quantum Chemistry
Web Portals
Coldfront
Helpdesk & Searchable Knowledgebase
WebMO
XDMoD Job Statistics
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for more info
See additional announcements in the Message of the
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Faculty Cluster Desktop - Advanced Options
Viz Node - CUDA Desktop
Viz Node - OpenGL Desktop
Jupyter Notebook
Host: >_cpn-p27-17
Created at: 2021-06-1
Time Remaining: 3 ho
Session ID: bbad5296
Connect to Jupyt
Faculty Cluster De
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
https://ondemand.ccr.buffalo.edu/pun/sys/dashboard/ba...ct/sys/bc_desktop/21-faculty_adv/session_contexts/new

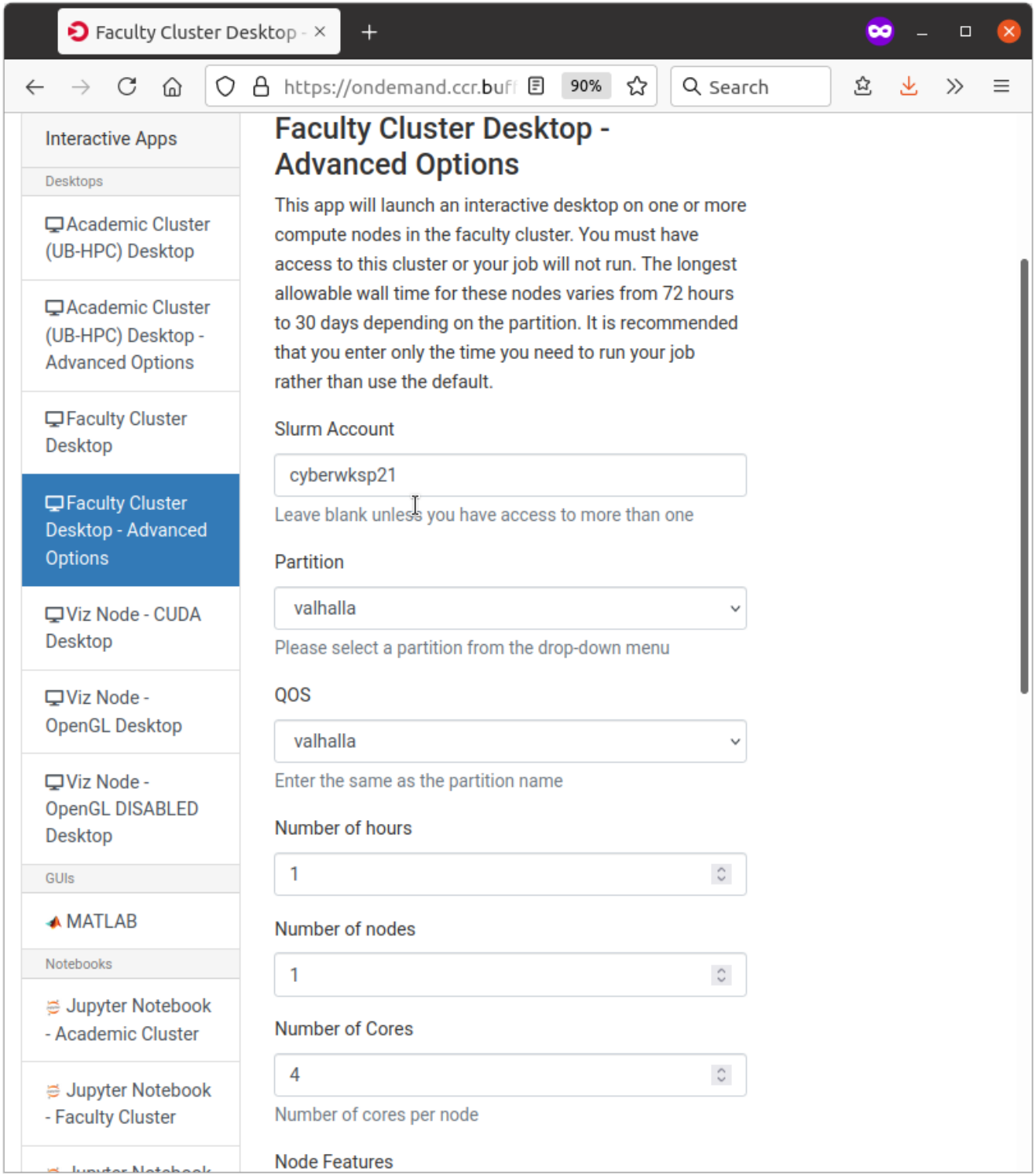
OnDemand Faculty Cluster App

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:


Faculty Cluster Desktop -
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Search
Interactive Apps
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Viz Node - CUDA Desktop
Viz Node - OpenGL Desktop
Viz Node - OpenGL DISABLED Desktop
GUIs
MATLAB
Notebooks
Jupyter Notebook - Academic Cluster
Jupyter Notebook - Faculty Cluster
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
cyberwksp21
Leave blank unless you have access to more than one
Partition
valhalla
Please select a partition from the drop-down menu
QOS
valhalla
Enter the same as the partition name
Number of hours
1
Number of nodes
1
Number of Cores
4
Number of cores per node
Node Features

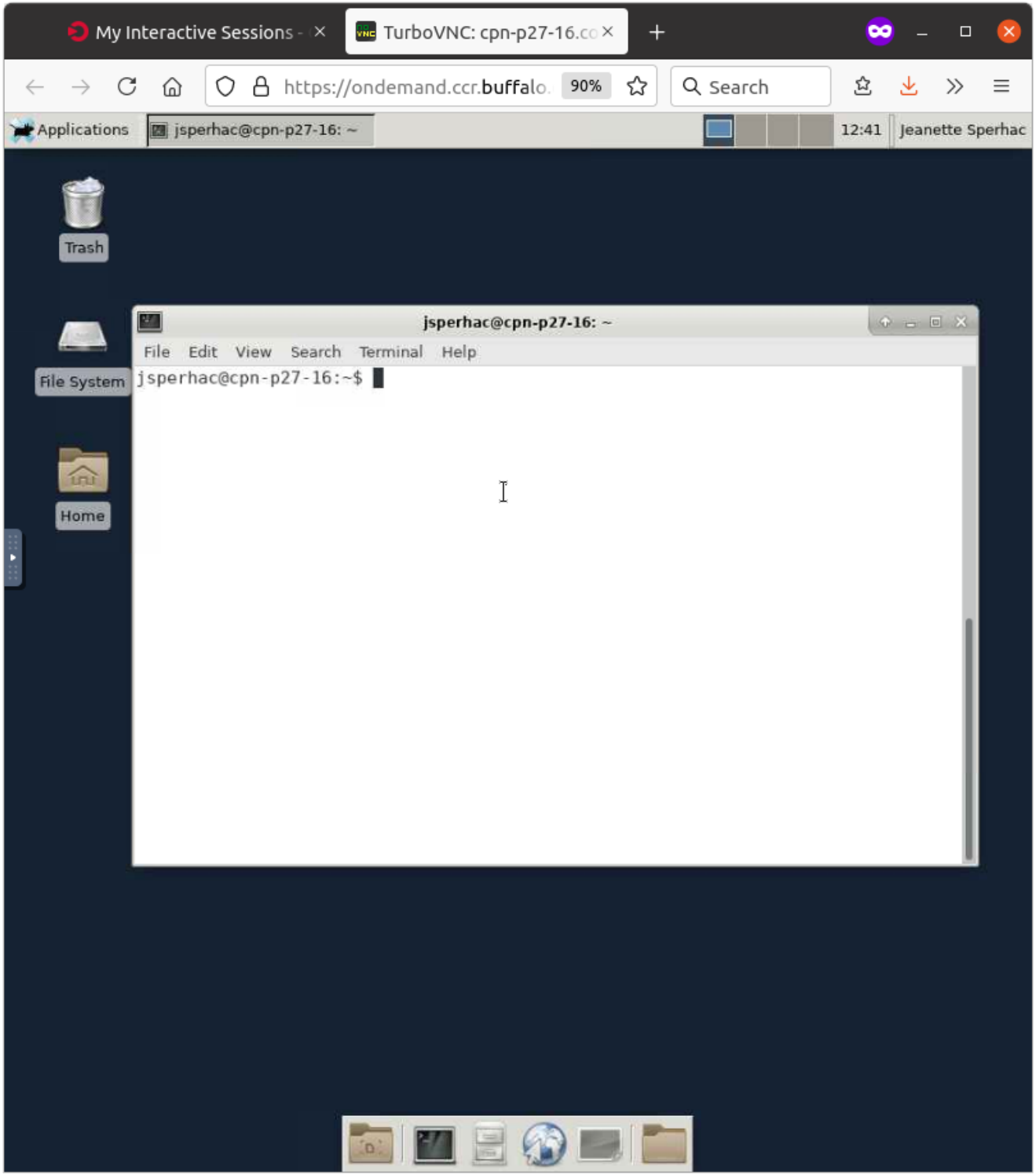
OnDemand Faculty Cluster App

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.cc
https://ondemand.ccr.buffalo.
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Applications
jsperhac@cpn-p27-16: ~
12:41
Jeanette Sperhac
Trash
File System
Home
jsperhac@cpn-p27-16: ~
File Edit View Search Terminal Help
jsperhac@cpn-p27-16:~$

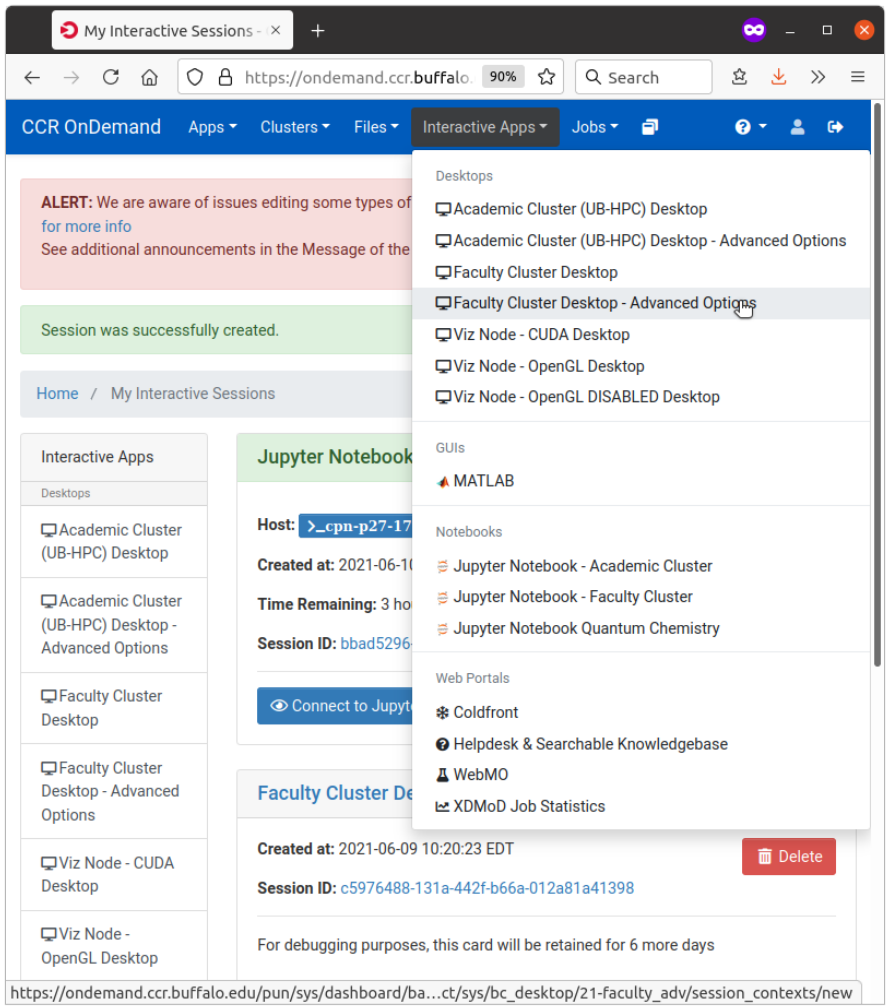
OnDemand Faculty Shell

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

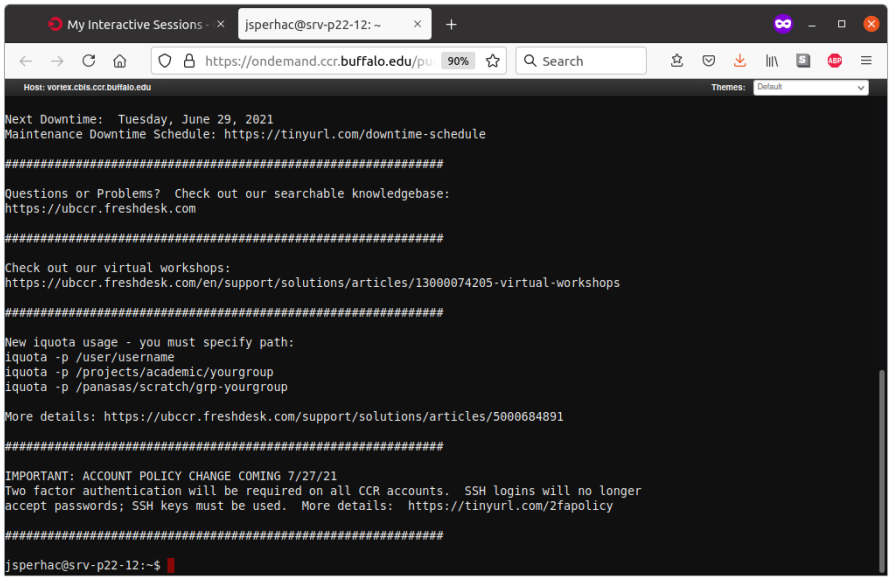
```
Clusters -> Faculty Cluster Shell Access
```

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:



2. Run the shell:

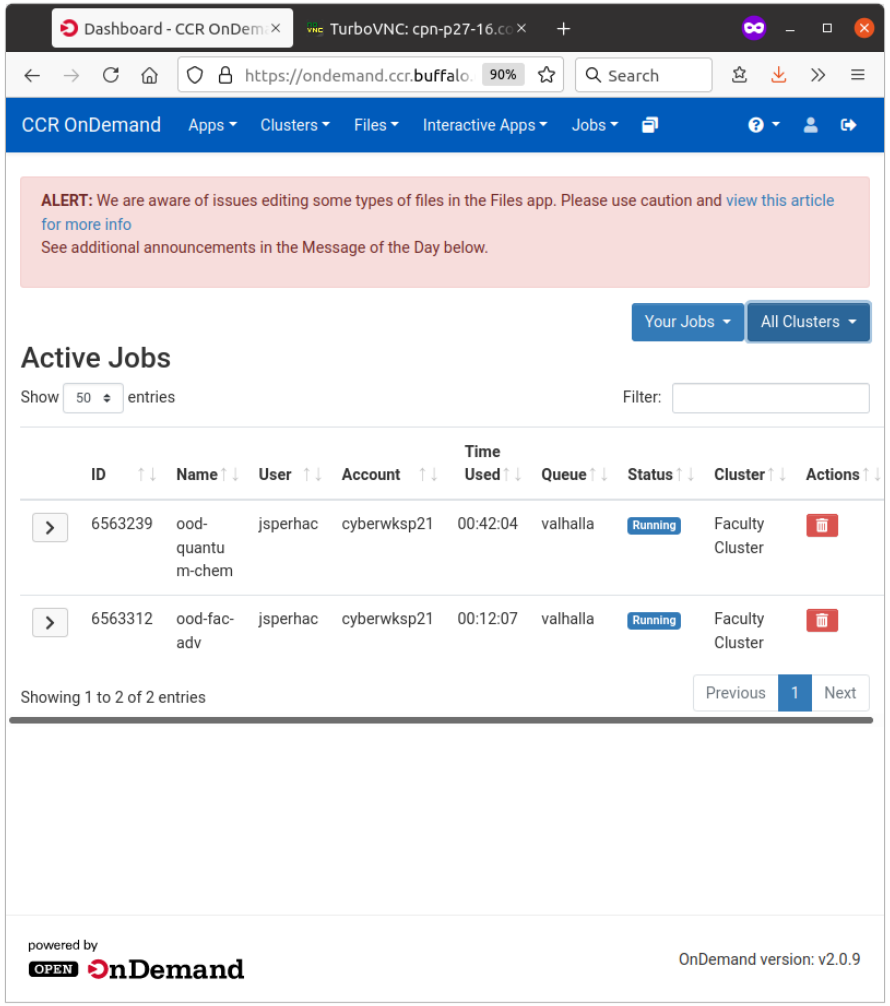


View your active jobs

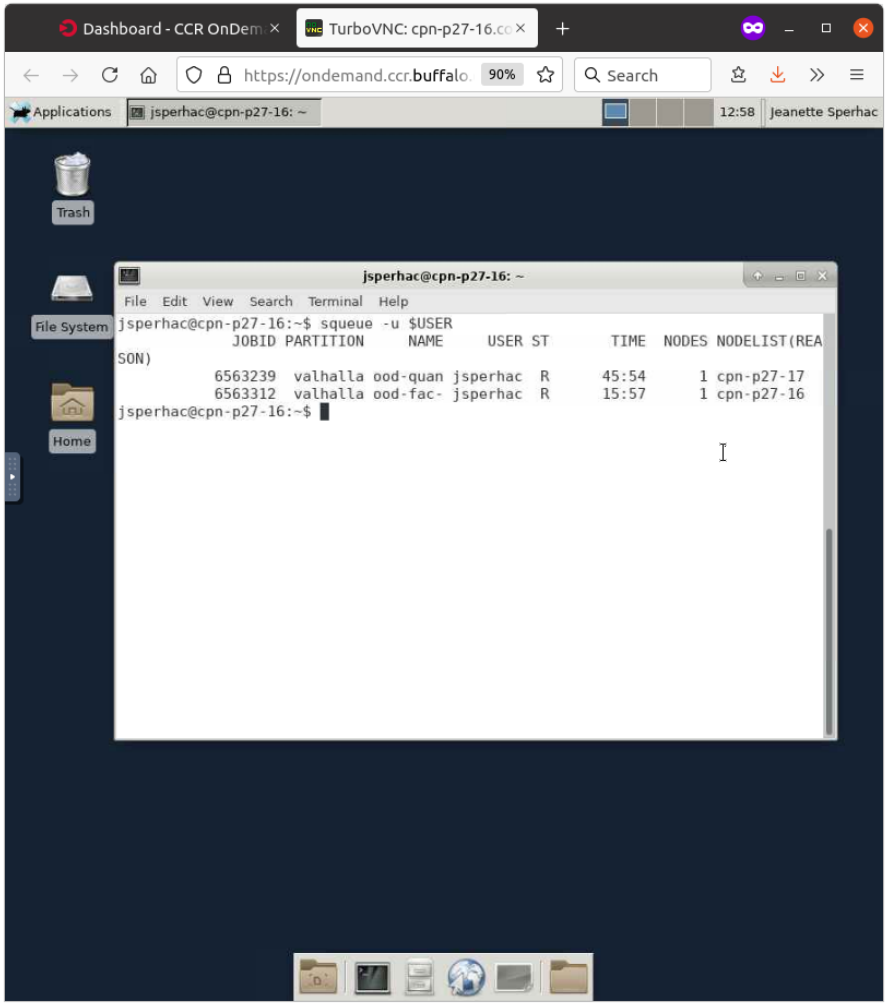
View jobs you are running right now:

```
Jobs -> Active Jobs
```

1. View in OnDemand:

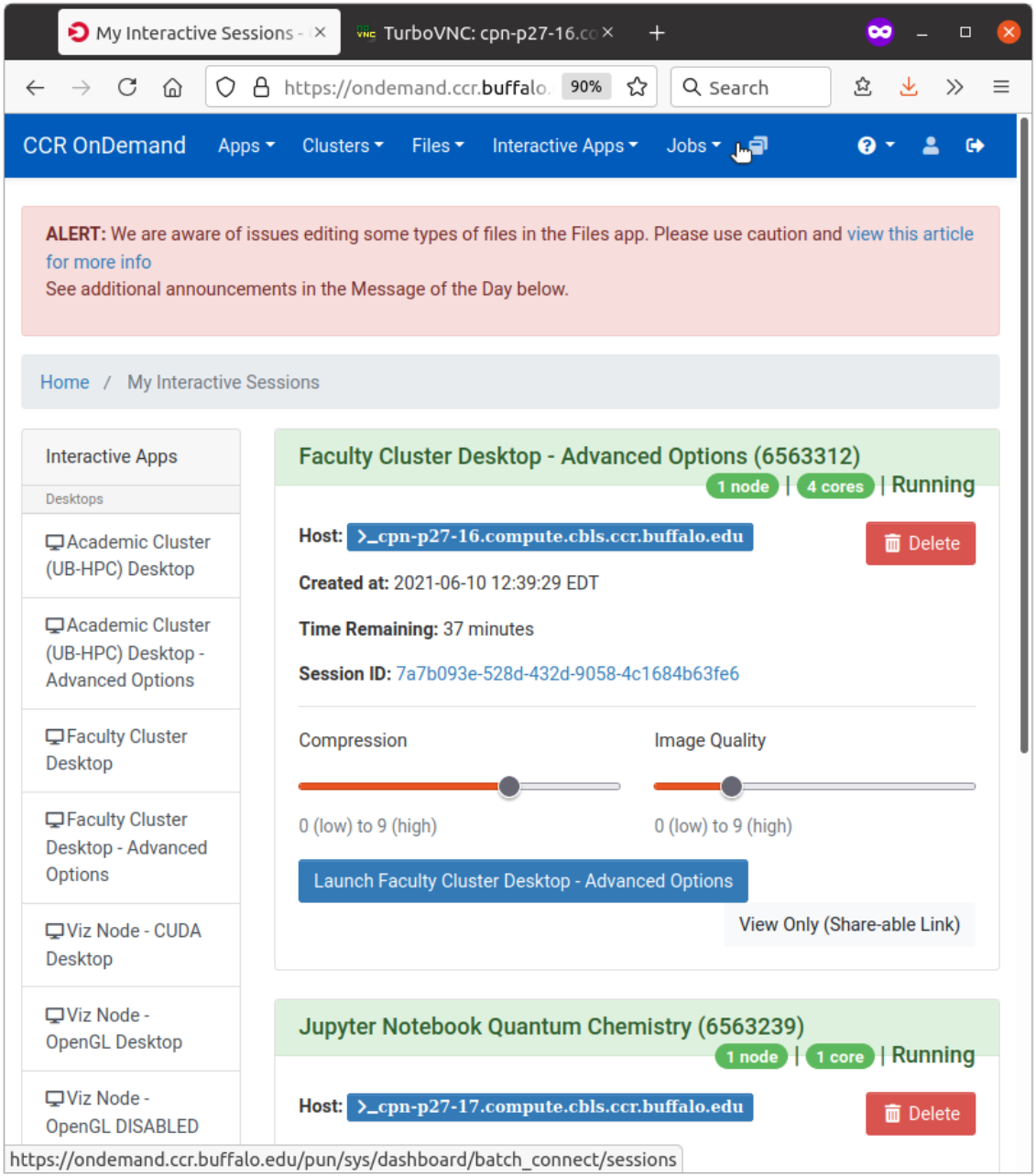


2. Or run squeue -u $USER in a terminal:



Troubleshoot and debug

View your OnDemand sessions (Click on the box icon, My Interactive Sessions):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TurboVNC: cpn-p27-16.co
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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.
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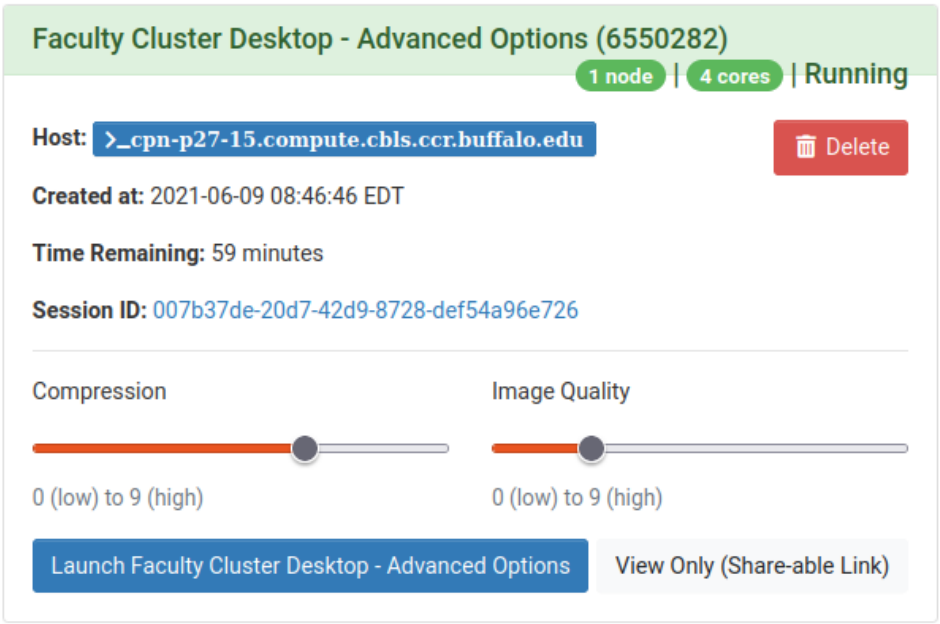
Academic Cluster (UB-HPC) Desktop - Advanced Options
Faculty Cluster Desktop
Faculty Cluster Desktop - Advanced Options
Viz Node - CUDA Desktop
Viz Node - OpenGL Desktop
Viz Node - OpenGL DISABLED
Faculty Cluster Desktop - Advanced Options (6563312)
1 node | 4 cores | Running
Host: >_cpn-p27-16.compute.cbls.ccr.buffalo.edu
Delete
Created at: 2021-06-10 12:39:29 EDT
Time Remaining: 37 minutes
Session ID: 7a7b093e-528d-432d-9058-4c1684b63fe6
Compression
Image Quality
0 (low) to 9 (high)
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

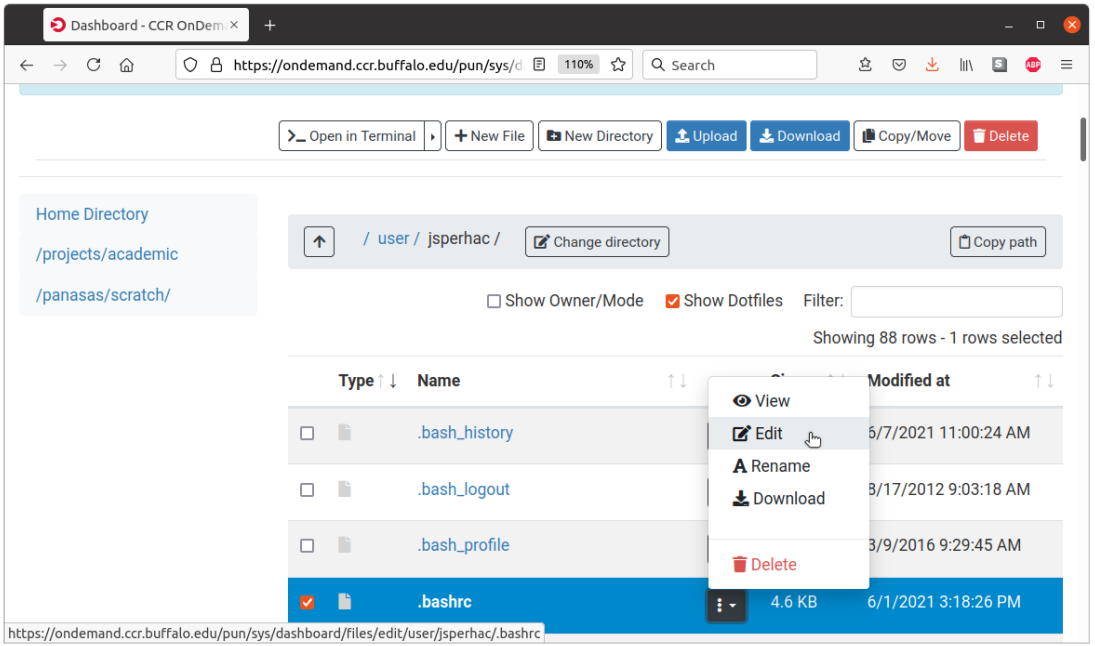
Troubleshoot and debug: zoom in on one session

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



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/