

Workshop setup at CCR

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Workshop checklist

Before the workshop begins, please ensure that you have followed emailed instructions from CCR to do the following:

- installed the UB VPN software on your own computer
- signed into the UB VPN software
- logged on to CCR and changed your CCR password
- verified your access to OnDemand at CCR

Quick Setup at CCR

This quick setup will prepare your account, settings, and directories for the workshop.

We will walk through these steps together during the workshop introduction session. Please carry them out in your own account!

Any problems, issues, or questions, please Slack or raise your hand.

Sign on

1. Connect to UB VPN (use your VPN password)
2. Sign in to OnDemand (use your CCR password):
<https://ondemand.ccr.buffalo.edu>.
3. In the OnDemand window, click Clusters -> Faculty Cluster Shell Access to open a shell, as shown:

Dashboard - CCR OnDem... File Editor - CCR OnDem... +

https://ondemand.ccr.buffalo.edu/pun/sys/d 110% Search

CCR OnDemand Apps Clusters Files Interactive Apps Jobs

- >_Academic Cluster Shell Access
- >_Faculty Cluster Shell Access
- >_Industry Cluster Shell Access

NEW USERS: Run this command in terminal to get shell access: `ssh -i /util/ccb/ssh_key/vortex.cbls.ccr.buffalo.edu -Y jobs: /util/ccb/bin/ssh_no_password.sh`

MACHINE STATUS: Check the status of the system, and **Faculty cluster status** or use 'sqstat'

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

VIRTUAL WORKSHOPS: Check out our library of virtual workshops [More info here](#)

FOLLOW US! CCR is on Twitter - [Get system status updates, helpful hints, & highlights of interesting research done at CCR](#)

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](#)

 **University at Buffalo**
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OnDemand provides an integrated, single access point for all of your HPC resources.

https://ondemand.ccr.buffalo.edu/pun/sys/shell/ssh/vortex.cbls.ccr.buffalo.edu

First time OnDemand access

You'll see a terminal as shown below. Use it to run this command:

```
/util/ccr/bin/ssh_no_password.sh
```

This ensures you can ssh between any nodes in the cluster. Keep your terminal open!

```
My Interactive Sessions - x jsperhac@srv-p22-12: ~ x +
https://ondemand.ccr.buffalo.edu/pu 90% Search
Host: vortex.cbis.ccr.buffalo.edu Themes: Default
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 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/2fapolicy
#####
jsperhac@srv-p22-12:~$
```

Link to project space

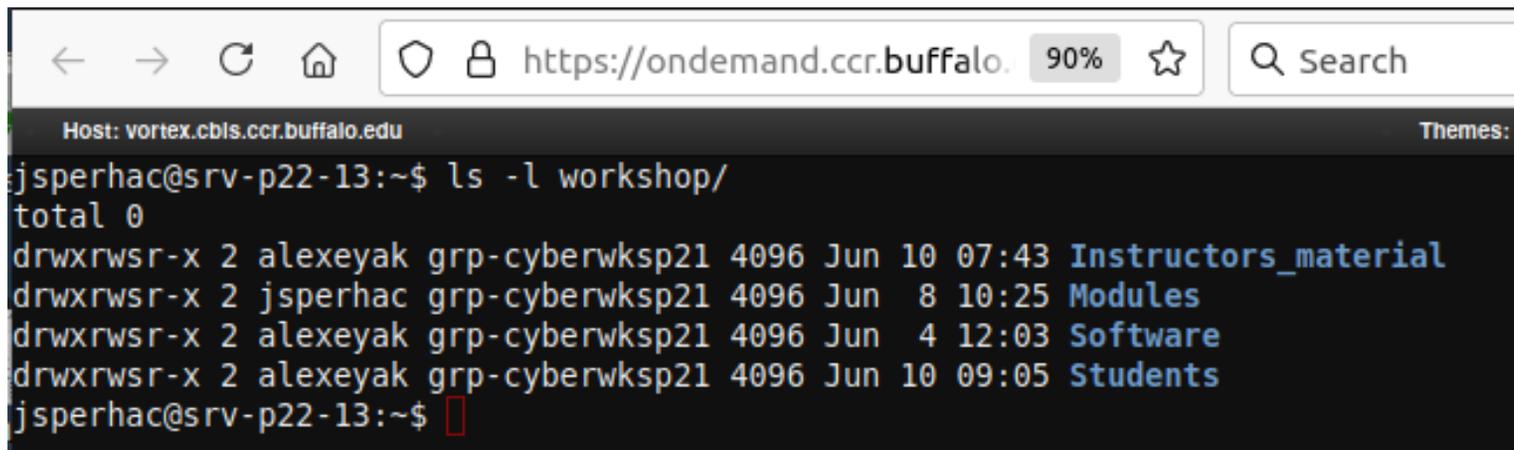
Next, in your terminal, create a link from your home directory to the project space by typing the following:

```
ln -s /projects/academic/cyberwksp21 ~/workshop
```

Check this by typing:

```
ls -l workshop
```

You should see something like this—a successful link to our project space:



```
Host: vortex.cbis.ccr.buffalo.edu Themes:
jsperhac@srv-p22-13:~$ ls -l workshop/
total 0
drwxrwsr-x 2 alexeyak grp-cyberwksp21 4096 Jun 10 07:43 Instructors_material
drwxrwsr-x 2 jsperhac grp-cyberwksp21 4096 Jun  8 10:25 Modules
drwxrwsr-x 2 alexeyak grp-cyberwksp21 4096 Jun  4 12:03 Software
drwxrwsr-x 2 alexeyak grp-cyberwksp21 4096 Jun 10 09:05 Students
jsperhac@srv-p22-13:~$
```

Create your project and scratch subdirectories

We now verify/create directories for your use during the workshop. These directories will have your own CCR username.

Verify your Student directory by typing:

```
ls /projects/academic/cyberwksp21/Students/ | grep $USER
```

...you will see your own username returned from this command.

Create your scratch directory by typing:

```
mkdir -p /panasas/scratch/grp-cyberwksp21/$USER
```

.bashrc edits

We now make two simple additions to your .bashrc file. You can use nano or vim editors for this task. We will demonstrate with nano.

From your home directory, type:

```
nano .bashrc
```

Use the arrow keys to move the cursor in nano. Add the following two lines to your .bashrc file:

```
module use /projects/academic/cyberwksp21/Modules  
export SLURM_CONF=/util/ccr/slurm/slurm-faculty.conf
```

Click ctrl-S to save, then ctrl-X to exit the nano editor. Then:

```
source .bashrc
```

Verify .bashrc

```
module avail
```

The first output returned should look like:

```
(base) jsperhac@srv-p22-13:~$ module avail
```

```
----- /projects/academic/cyberwksp21/Modules -----  
columbus      dftbplus      eqe            ergoscf-mpi    lammps         nx            qxmd  
cp2k          (L)          dynemol       ergoscf        jupyter       (L)          nexmd         qe
```

Congratulations

You're ready for the workshop!