SAVIO cluster

Register new accounts

- 1. create portal accounts at MyBRC User Portal (https://mybrc.brc.berkeley.edu/)
- 2. After following the on-screen instructions in the portal and registering and/or logging in, you should first review and sign the cluster <u>User Access Agreement Form</u> on the Home ("Welcome") page (if they haven't already done so from within the portal previously) by clicking on the "Review" button
- 3. Click on the "Join" button to request to join project, you can search ic_chem242 under project name to find our class project. Click on "join".
- 4. We will approve your request. And for new users there will be a processing wait time of a few days or so between the time they join their first project via the MyBRC User Portal and the time they receive the confirmation email pointing them to instructions on how they can access their new BRC user account.

From Terminal (You'll need do this first to setup the kernel)

You only need to do this once.

- Log into cluster
 - 1. ssh your user name@hpc.brc.berkeley.edu
 - 2. fill in your password and OTP in one entry
 - 3. Run the following command (in one line) to create a symlink from the kernel I set to your directory:

 $ln \hbox{--}s \hbox{--}nancy_guan/.local/share/jupyter/kernels/pt 10$

- ~ your user name/.local/share/jupyter/kernels/pt10
- 4. Then run the following command and make sure you can see kernel pt10.

jupyter kernelspec list

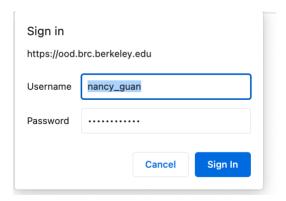
Available kernels:

0 /global/home/users/nancy_guan/.local/share/jupyter/kernels/pt10

5. Now you can proceed with the next session to run interactive notebooks.

From Server (for interactive jupyter notebooks)

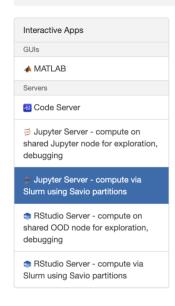
- 1. Go to ood.brc.berkeley.edu
- 2. You'll be taken to a sign in page. Fill in username, password and OTP here. OTP is a 6-digit one-time password (from Google Authenticator)



3. You should see this page, and then select interactive apps – Jupyter Server Savio partitions



4. Fill in the information as shown below to request an interactive node. You can change the wall clock time to the number of hours you need.



Jupyter Server - compute via Slurm using Savio partitions version: 2021.pumpkin-2-g42a194c

This app will launch a Jupyter server session on the Berkeley Research Computing(BRC) Savio cluster.

Name of the Job

OOD_Jupyter

SLURM Partition

savio2_gpu

The SLURM Partition in which you want to launch this Jupyter session.

SLURM Account/Project Name

ic_chem242

The SLURM account (i.e., the value of the -A or --account flag used when submitting a SLURM job).

SLURM QoS Name

savio_normal

The QoS you want run under. Most FCA users choose savio_normal. Condo users can either use their condo QoS or the low-priority QoS.

Number of Compute Nodes

1

The number of nodes you want for your Jupyter session.

Number of CPU Cores per Node

2

The number of CPU cores you want per node for your Jupyter session.

Number and Type of GPUs

gpu:1

The GRES value in the form 'gpu:x' or 'gpu:type:x' where 'x' is the number of GPUs and (optionally) 'type' is the type of GPU. Remember to specify two CPUs for each GPU in the 'Number of CPU Cores per Node' field.

Wall Clock Time

2

The maximum number of hours your Jupyter session will run for. To save FCA credits or free up resources for your condo group members, you should delete your session when you are done.

Email Address (Optional)

Enter your email address if you would like to receive an email when the session starts. Leave blank for no email.

Launch

^{*}The Jupyter Server - compute via Slurm using Savio partitions session data for this session can be accessed under the data root directory.

5. You should see this page when the node is ready. Click on Connect to Jupyter. If you finish earlier than the time you requested, you can click on Delete to free up the node for other people.



6. You are now on the Jupyter Server! You can upload files here or start a new notebook. You should see a kernel with name Python3.6 PT1.0.0 after you follow previous steps to set up a symlink, which allows you to import pytorch.



File Transfer

https://docs-research-it.berkeley.edu/services/high-performance-computing/userguide/data/transferring-data/using-scp-savio/

Run these commands from your local terminal

- Download.
 - scp your_user_name@dtn.brc.berkeley.edu:/remote/path/myfile /local/path
- o Upload.
 - scp /local/path/myfile your_user_name@ dtn.brc.berkeley.edu:/remote/path
- Use **scp -r** for transferring folders.
- The remote path needs to be inside your \$HOME folder, you can find this path by running **pwd** after log into cluster. In general it should look like /global/home/users/your_user_name