Lawrencium 101: HPC on Lawrencium Supercluster

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HPCS User Support Team

Outline

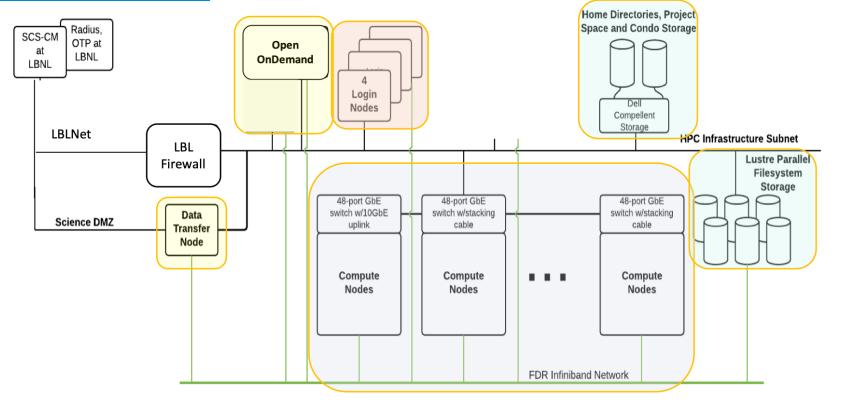
- 1. Overview of Lawrencium supercluster
- 2. Getting Access and login to cluster
- 3. Data transfer to/from clusters
- 4. Software access and installation
- 5. Job submission and monitoring
- 6. Open On Demand: a browser based HPCS portal

Overview of Lawrencium supercluster

- A LBNL Condo Cluster Computing Program
 - Support researchers in all disciplines at the Lab
 - Significant investment by the IT division
 - Individual PIs buy in compute nodes and storage
 - Computational cycles are shared among all lawrencium users
- Lawrencium Compute Nodes
 - data center is housed in the building 50B
 - over 2187 compute nodes (~65016 CPU cores)
 - 210 GPU cards
 - 32 partitions, lr3, lr4, lr5,lr6, es1, cm1 ...
 - 1652 user accounts
 - 410 projects/groups

Conceptual Diagram of Lawrencium



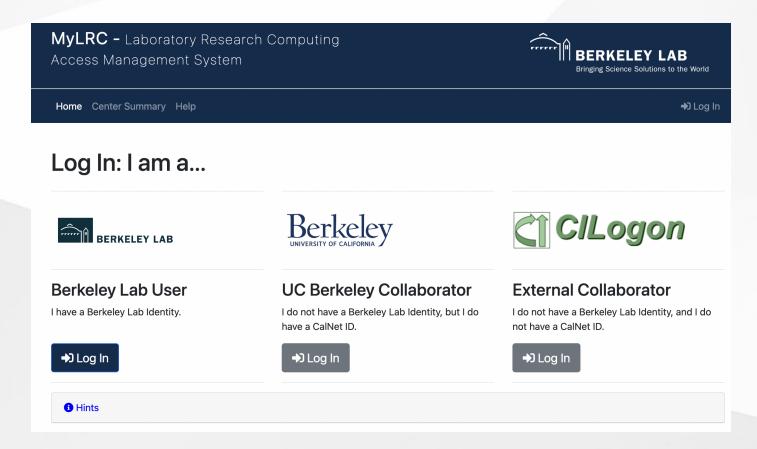


Quick Poll:

Check poll question and chose your answer here and enter your answer.

Getting Access to Cluster: MyLRC User portal

The form based request for project and user accounts are now moved to MyLRC portal



Want to learn more about MyLRC portal? Join HPCS trainign on 7th February.

Getting Project Accounts

- Three types of project accounts can be requested.
 - 1. Primary Investigator (PI) Computing Allowance (PCA) account: free 300K service units (SUs) per year (pc_xxx)
 - 2. **Condo account**: Pls buy in compute nodes to be added to the general pool, in exchange for their own priority access and share the Lawrencium infrastructure (lr_xxx)
 - 3. **Recharge account**: pay as you go with minimal recharge rate ~ \$0.01/SU (ac_xxx)
- Check out more details here. <u>Project Accounts</u>
- LBL affiliated PI can request project accout at MyLRC portal
- PIs can grant PCA/condo/recharge project access to researchers/students and external collaborators.

Getting User Accounts

- PIs can sponsor researchers/students and external collaborators for cluster accounts.
- Account requests and approval will be done through <u>MyLRC portal</u>.
- Workflow
 - Account creation request on the MyLRC portal
 - Automatic email is sent to PI for approval
 - PI approves request on the MyLRC portal
 - Account creation on the cluster by HPCS team
 - Users are notified upon account availability and OTP setup.
- Check out <u>documentation</u>.
 - Help us build <u>FAQ</u>. Submit your questions <u>here</u>.

Login to Lawrencium Cluster

- Linux: Terminal (command-line) session.
- Mac: Terminal (see Applications -> Utilities -> Terminal).
- Windows: PowerShell, or PuTTY or MobaXterm.
- One-time passwords (OTPs): set up Google Authenticator app on your smartphone or tablet <u>Instructions Here</u>
- Login:

```
ssh $USER@lrc-login.lbl.gov
password:
```

• Password: your 4-digit PIN followed by 6-digit one-time password from your Google Authenticator. Example PIN: 0123 OTP: 456789.

```
password:0123456789
```

Note: Characters won't appear on a screen in the password prompt when you enter in the digits.

FAQ: What if I forget my PIN?

--> Reset PIN and test PIN+OTP here.

Login to Lawrencium Cluster

Upon login to Lawrencium, you'll end up on one of the login nodes in your home directory.

```
spsoni@n0000 ~]$ hostname
n0000.scs00
[spsoni@n0000 ~]$ pwd
/global/home/users/spsoni
[spsoni@n0000 ~]$
```

DO NOT run jobs on login nodes!!

User Spaces

- Home: /global/home/users/\$USER/ 20GB per user, data is backed up, recommended for keeping scripts and final results data
- Global Scratch: /global/scratch/users/\$USER/, shared, no backup, high performance Lustre parallel filesystem, recommended for keeping non-persistent data for computation.
- Shared group project space
 - /global/home/groups-sw/ Size: 200GB, backup: YES
 - /global/home/group/ Size: 400GB, backup: NO
- Condo Storage:
 - e.g. /clusterfs/etna/ or /global/scratch/projects/xxx

Data Transfer

Irc-xfer.lbl.gov: Data Transfer Node (DTN)

• On Linux: scp/rsync

```
# Transfer file or directory from a local machine to Lawrencium
scp file-xxx $USER@lrc-xfer.lbl.gov:/global/home/users/$USER
scp -r dir-xxx $USER@lrc-xfer.lbl.gov:/global/scratch/users/$USER

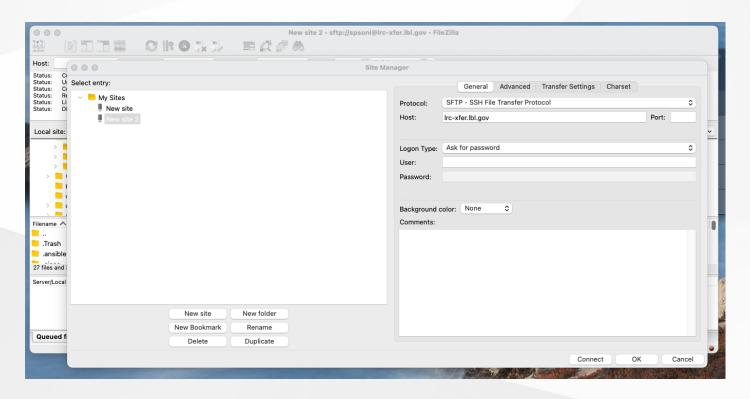
# Transfer file or directory from Lawrencium to a local machine
scp $USER@lrc-xfer.lbl.gov:/global/scratch/users/$USER/file-xxx ~/Desktop
scp -r $USER@lrc-xfer.lbl.gov:/global/scratch/users/$USER/dir-xxx ~/Desktop
# Transfer directory from Lawrencium to Another Institute
ssh $USER@lrc-xfer.lbl.gov # DTN
scp -r $USER@lrc-xfer.lbl.gov:/dir-on-lawrencium $USER@other-institute:/destination/path/$USER

rsync: a better data transfer or a backup tool
rsync -avpz file-at-local $USER@lrc-xfer.lbl.gov:/global/home/users/$USER
```

- On Window
 - WinSCP: SFTP client and FTP client for Microsoft Windows
 - FileZilla: multi-platform program via SFTP

FileZilla

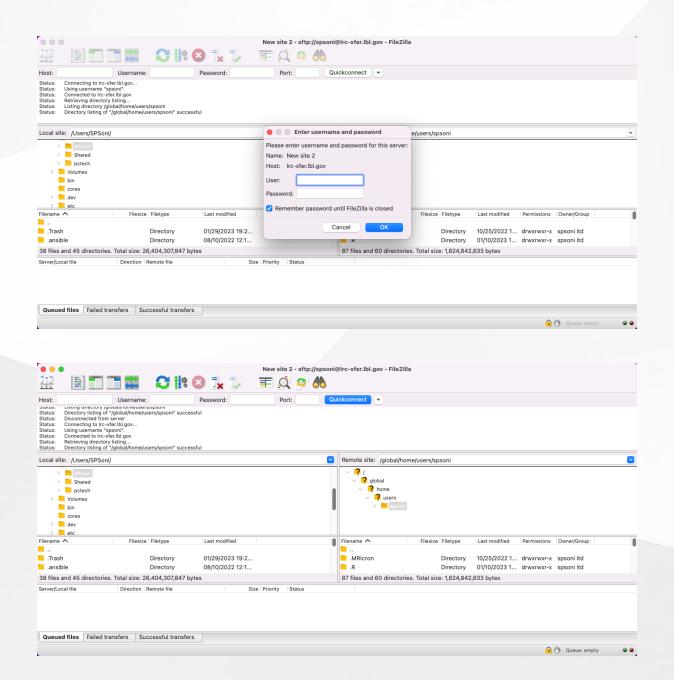
Site Manager (on the top right corner)



Click on connect to access Lawrencium for file transfer.

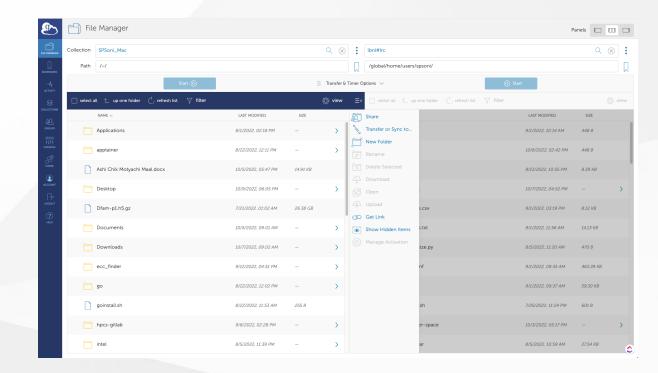
Enter your username and password (LRC credentials) in the pop-up window.

Once the connection is established, you are ready to drag and drop files to/from lawrencium.



Data Transfer with Globus

- Globus can be used for fast data transfer and sharing with collaborators. Connect to globus https://globus.lbl.gov
- Globus for Lawrencium
- Berkeley Lab users can use Globus to transfer files in/out of their LBNL Google drive.
- Possible endpoints include: Ibnl#Irc, ucb#brc, your laptop/desktop, NERSC.
- Transfer data to/from your laptop (endpoint setup)
 - Create an endpoint on your machine using Globus Connect Personal globusconnect-personal
 - Run Globus Connect Pesonal on your local machine



Software Access: Software Module Farm

- Software stack, commonly used compiler, software tools are provided to all users through <u>software</u> <u>module farm on lawrencium</u>
- Installed and maintained on a centralized storage device and mounted as read-only NFS file system
 - Compilers: e.g. intel, gcc, MPI compilers, Python
 - Tools: e.g.matlab, singularity/apptainer, cuda
 - Applications: e.g. machine learning, QChem, MD, cp2k
 - Libraries: e.g. fftw, lapack

Environment Modules

- Manages users' software environment by dynamically setting up \$PATH, \$LD_LIBRARY_PATH...
- Avoid clashes between incompatible software versions

```
module purge: clear user's work environment
module available: check available software packages
module load packagename/version: load a package
module list: check currently loaded software
```

- Modules are arranged in a hierarchical fashion, some of the modules become available only after the parent module(s) are loaded
- e.g., MKL, FFT, and HDF5/NetCDF software is nested within the gcc module
- Example: load an OpenMPI package

```
module available openmpi mkl
module load intel/2016.4.072
module av openmpi
module load mkl/2016.4.072 openmpi/3.0.1-intel
```

Software Installation

- Users can install software in their home, scratch or group space. Packages installed in group space are accessisble to all group memebers.
- Users don't have admin rights, but most software can be installed at custom path using
 --prefix=/path/to/your/dir

Installing Python Packages as an example case

- Python modules: abundantly available but cannot be installed in the default location without admin rights.
- pip install --user package_name
- export PYTHONPATH=~/.local/lib/pythonX.X/site-packages/\$PYTHONPATH

```
[spsoni@n0000 ~]$ module load python/3.9.12
[spsoni@n0000 ~]$ python3 -m site --user-site
/global/home/users/spsoni/.local/lib/python3.9/site-packages
[spsoni@n0000 ~]$ pip install --user ml-python
...
Successfully built ml-python
Installing collected packages: ml-python
Successfully installed ml-python-2.2
[spsoni@n0000 ~]$ export PYTHONPATH=~/.local/lib/python3.9/site-packages/$PYTHONPATH
```

- pip install: --install-option="--prefix=\$HOME/.local" package_name
- Install from source code: python setup.py install --prefix=/home/user/package_dir
- Create a virtual environment: python -m venv my_env
 - Activate environment: source my_env/bin/activate
 - Install packages into it: python -m pip install <package-name>
 - Deactivate environment: deactivate
- Conda environment: conda create -p /global/scratch/users/spsoni/my_env <package-name>
 - Activate environment: source activate /global/scratch/users/spsoni/my_env
 - Deactivate environment: conda deactivate

Job Submission and Monitoring: SLURM

SLURM is the resource manager and job scheduler for managing all the jobs on the cluster.

Why is this necessary?

- Prevent users' jobs running on the same nodes.
- Allow everyone to fairly share Lawrencium resources.

Basic workflow:

- login to Lawrencium; you'll end up on one of the login nodes in your home directory
- cd to the directory from which you want to submit the job (scratch recomended)
- submit the job using sbatch or an interactive job using srun (discussed later)
- SLURM assign compute node(s) to your jobs
- your jobs will run on a compute node, not the login node

Accounts, Partitions, Quality of Service (QOS)

Check slurm association, such as qos, account, partition, the information using following command.

This information is required when submitting a job. For Lawrencium cluster information click here

Interactive Job Submission

Interactive job submission is typically used for code debugging, testing, monitoring.

- **srun**: add your resource request to the queue.
- When the allocation starts, a new bash session will start up on one of the granted nodes

```
• srun --account=ac_xxx --nodes=1 --partition=lr5 --qos=lr_normal --time=1:0:0 --pty bash
```

• srun -A ac_xxx -N 1 -p lr5 -q lr_normal -t 1:0:0 --pty bash

Once you are on the assigned compute node, start application/commands directly

- **salloc**: similarly to *srun* --pty bash
- a new bash session will start up on the compute node, -pty gives you a pseudo terminal

Node Features

Compute nodes may have different hardware within a SLURM partition, e.g. LR6 - Ir6_sky: Intel Skylak, Ir6_cas: Intel Cascade Lake, Ir6_cas,Ir6_m192: Ir6_cas + 192GB RAM, Ir6_sky,Ir6_m192: Ir6_sky + 192GB RAM

- Lawrencium nodes features can be found here.
- wait time is longer when a specific type of node is requested
- Slurm flag: --constrain

```
[spsoni@n0000 ~]$ srun --account=scs --nodes=1 --partition=lr6 --time=1:0:0 --qos=lr_normal --constrain=lr6_sky --pty bash
[spsoni@n0081 ~]$ free -h
                                                 shared buff/cache
                                                                       available
              total
                           used
                                       free
Mem:
                93G
                           2.2G
                                        83G
                                                   3.1G
                                                               7.4G
                                                                             87G
               8.0G
                             0B
                                       8.0G
Swap:
[spsoni@n0081 ~]$ exit
exit
```

Memory Specification

- Most Lawrencium partitions are exclusive: a compute node allows only one user
- Some condo accounts or partitions, such as es1 (GPUs), each compute node can be shared by multiple users
- Slurm flag: --mem (MB) is required when using a shared partition:
- e.g. a compute node with 96GB RAM, 40 core node: 2300 RAM/core
 - --ntask=1 --mem=2300 (request one core)
 - --ntask=2 --mem=4600 (request 2 cores)
- LR6 partition lr_bigmem: two large memory nodes (1.5TB)
- Slurm flag: --partition=lr_bigmem

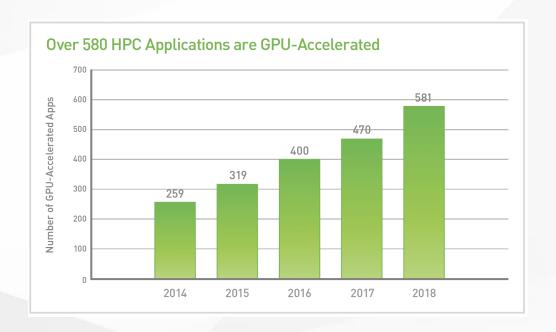
Batch Job Submission

- Get help with the complete command options sbatch --help
- sbatch: submit a job to the batch queue system sbatch myjob.sh
- Download batch job scripts <u>here</u>.

myjob.sh: Job submission script for serial job

```
#!/bin/bash
#SBATCH --job-name=mytest # Job name
#SBATCH --partition=lr6
                            # Partition
#SBATCH --account=pc_test
                            # Account, replace it with your own account allocation
#SBATCH --qos=lr_normal
                            # qos
#SBATCH --time=1:00:00
                            # Wall clock time
#SBATCH --nodes=1
                            # Node count
#SBATCH --constrain=lr6_cas
#SBATCH --mail-user=xxx@lbl.gov
##SBATCH --mail-type=BEGIN/END/FAIL
#SBATCH --mail-type=ALL
# cd to your work directory
cd /your/dir
## Commands to run
module load python/3.9.12
python my.py >& mypy.out
```

Do you want to accelerate computation to gaming speed??



GPU: Graphical Processing Units, Image Credits: NVIDIA blog

Common Scientific packages: GAMESS, NAMD, LAMMPS, GROMACS, Gaussian, VASP, Amber, GAMESS, Quantum Expresso, BLAST, ANSYS, LS-DYNA Lawrencium cluster's **es1 partition** provides nodes with 2080Ti, V100 and A40 GPUs.

Submit Jobs to es1 GPU Partition

- --gres=gpu:type:GPU#
- --ntasks=CPU_CORE#
- ratio CPU_CORE#:GPU# = 2:1

```
[spsoni@n0000 ~]$ srun -A scs -N 1 -p es1 --gres=gpu:1 --ntasks=2 -q es_normal -t 0:30:0 --pty bash
[spsoni@n0022 ~]$ nvidia-smi
Mon Oct 10 16:17:49 2022
 NVIDIA-SMI 460.84
                  Driver Version: 460.84
                                       CUDA Version: 11.2
-----+
             Persistence-M| Bus-Id
                                  Disp.A | Volatile Uncorr. ECC
 Fan Temp Perf Pwr:Usage/Cap|
                              Memory-Usage | GPU-Util Compute M.
0 Tesla V100-SXM2... Off | 00000000:62:00.0 Off |
                                                      0
                           0MiB / 16160MiB |
          P0 52W / 300W I
                                            0%
                                                  Default
                                                     N/A
  1 Tesla V100-SXM2... Off | 00000000:89:00.0 Off |
                                                      0
 N/A 43C
               54W / 300W |
                           0MiB / 16160MiB |
                                                  Default
 Processes:
                                                GPU Memory
 GPU GI CI
                    Type
                          Process name
                                                Usage
______
 No running processes found
```

- Specify GPU type : --gres=gpu[type]:count
 - GRTX2080TI(GPU count = 3 or 4): --gres=gpu:GRTX2080TI:1
 - V100(GPU count = 2): --gres=gpu:V100:1
 - A40(GPU count = 4): --gres=gpu:A40:1
- In above example only one gpu is used but count can be set to total number of GPUs at the max.

```
[spsoni@n0000 ~]$ srun -A scs -N 1 -p es1 --gres=gpu:V100:2 --ntasks=4 -q es_normal -t 0:30:0 --pty bash

[spsoni@n0016 ~]$ nvidia-smi -L

GPU 0: Tesla V100-SXM2-16GB (UUID: GPU-7979861e-e0ad-000f-95fb-371e34593991)

GPU 1: Tesla V100-SXM2-16GB (UUID: GPU-50d24ac9-9eea-f96b-cc8b-db849f9c9427)

[spsoni@n0016 ~]$ echo $CUDA_VISIBLE_DEVICES

0,1
```

Submit A GPU Batch Job

myjob_gpu.sh: Job Submission Script for GPUs

```
#!/bin/bash -1
#SBATCH --job-name=mytest
#SBATCH --partition=es1
                                ## es1 GPU partition
#SBATCH --account=pc_test
#SBATCH --qos=es_normal
                                ## qos of es1
#SBATCH --time=1:00:00
#SBATCH --nodes=1
#SBATCH --gres=gpu:V100:2
                               ## GPUs
#SBATCH --ntasks=4
                               ## CPU cores
#cd /your/dir
#Number of GPUs, this can be in the format of "gpu:[1-4]", or "gpu:V100:[1-2] with the type included
## Commands to run
module load ml/tensorflow/2.5.0-py37
python tf.py >& tf.out
```

Submiting MPI Jobs

When using multiple nodes, you need to carefully specify the resources. The key flags to use in your job script are:

- --nodes or -N: number of nodes
- --ntasks-per-node: number of tasks (i.e., processes) to run on each node, especially useful when your job uses large memory, < Max Core# on a node
- --ntasks or -n: total number of tasks and let the scheduler determine how many nodes and tasks per node are needed.
- --cpus-per-task : number of cpus to be used for each task

Submiting MPI Jobs

myjob_mpi.sh: Job submission script

```
#!/bin/bash
#SBATCH --job-name=test_mpi
#SBATCH --account=pc_test
#SBATCH --partition=lr6
#SBATCH --qos=lr_debug
#SBATCH --ntasks=40 # Number of MPI tasks needed for use case (example):
#SBATCH --nodes=2 # Nodes count
##SBATCH --ntasks-per-node=20 ## important with large memory requirement

# Wall clock limit:
#SBATCH --time=00:01:30
## Command(s) to run (example):
module load gcc/11.3.0 openmpi/4.1.4-gcc
srun ./hello >& hello.out
```

Submit Serial Tasks in Parallel (GNU Parallel)

GNU Parallel is a shell tool for executing jobs in parallel on one or multiple computers.

- A job can be a single core serial task, multi-core or MPI application.
- A job can also be a command that reads from a pipe.
- Typical input:
 - bash script for a single task
 - a list of tasks with parameters
- Example Using GNU Parallel

Bioinformatics tool *blastp* to compare 200 RNA query sequences against sequence DB Serial bash script: **run-blast.sh**

```
[spsoni@n0003 gnu_parallel]$ cat run-blast.sh
#!/bin/bash
module load bio/blast/2.13.0
module load parallel/20200222
blastn -db database/16S_ribosomal_RNA -query $1 -out $2 -task blastn -dust no -outfmt "7 \
delim=, qacc sacc evalue bitscore qcovus pident" -max_target_seqs 5
```

task.lst: each line provides one parameter to one task:

```
[spsoni@n0003 gnu_parallel]$ cat task.lst
data/query1.fa
data/query2.fa
.
data/query200.fa
```

Instead submit single core-jobs 200 times, which potentially need 200 nodes, GNU parallel sends single-core jobs in parallel using all the cores available, e.g. 2 compute nodes 32*2=64 parallel tasks. Once a CPU core becomes available, another job will be sent to this resource.

myjob_gnuparallel.sh: Slurm script for gnu-parallel job submission on lawrencium

```
#!/bin/bash
#SBATCH --job-name=test_gnupar
#SBATCH --account=pc_test
#SBATCH --partition=lr6
#SBATCH --qos=lr_normal
#SBATCH --nodes=2
#SBATCH --time=2:00:00
## Command(s) to run (example):
module load bio/blast/2.13.0
module load parallel/20200222
export WORKDIR=/global/scratch/users/spsoni/LRC101/gnu_parallel
cd $WORKDIR
echo $SLURM_JOB_NODELIST |sed s/\,/\\n/g |awk -v cores=$SLURM_CPUS_ON_NODE '{print cores"/"$1}' > hostfile
mkdir -p output logs
export JOBS_PER_NODE=32
parallel --jobs $JOBS_PER_NODE --slf hostfile --wd $WORKDIR --joblog task.log --progress -a task.lst sh run-blast.sh {} output/{/.}.blst
```

Host file will be generated at run time by the above script.

Detailed information of how to submit serial tasks in parallel with GNU Parallel

Job Monitoring

• sinfo: check node status of a partition (idle, allocated, drain, down)

```
[spsoni@n0000 \sim]$ sinfo -r -p 1r5
PARTITION AVAIL TIMELIMIT NODES STATE NODELIST
1r5
                 infinite
                              3 drain* n0004.lr5,n0032.lr5,n0169.lr5
            up
                infinite 14
1r5
                                  down n0048.1r5,n0050.1r5
            up
                                alloc n0000.1r5,n0001.1r5,n0002.1r5,n0003.1r5,n0006.1r5,n0009.1r5
1r5
                 infinite
            up
                 infinite
                                  idle n0005.1r5,n0007.1r5,n0008.1r5
                          115
lr5
            up
```

• **squeue**: check job status in the batch queuing system (R or PD)

```
squeue -u $USER
             JOBID PARTITION
                                 NAME
                                         USER ST
                                                        TIME NODES NODELIST(REASON)
          28757187
                                 bash spsoni R
                                                      0:09
                                                                1 n0215.1r6
                         1r6
                                 bash spsoni R
                                                      0:16
          28757723
                                                                1 n0002.es1
                         es1
                                 bash spsoni PD
                                                              120 (QOSMaxNodePerJobLimit)
          28759191
                         lr6
                                                      0:00
```

• sacct: check job information or history

ı	[spsoni@n0002 JobID		-j 28757723 Partition	Account	AllocCPUS	State	ExitCode
1	28757723	bash	es1	scs	2	RUNNING	0:0
1	[spsoni@n0002	~]\$ sacct	-X -o 'jobio	d,user,part:	ition,nodel:	ist,stat'	
ı	JobID	User	Partition	NodeL:	ist St	ate	
	28755594	spsoni	lr5	n0192.lr5	COMPLETED		
	28755597	spsoni	lr6	n0101.lr6	COMPLETED		
	28755598	spsoni	lr5	n0192.lr5	COMPLETED		
	28755604	spsoni csd_	_lr6_s+	n0144.lr6	COMPLETED		
	28755693	spsoni	lr6	n0101.lr6	CANCELLED+		
	28757187	spsoni	lr6	n0215.lr6	COMPLETED		
	28757386	spsoni	es1	n0019.es1	FAILED		
	28757389	•	es1	n00073.cs1			
		spsoni					
	28757723	spsoni	es1	n0002.es1	RUNNING		

wwall -j <JOB_ID>: check resources utilization of an active job from a login node

```
[spsoni@n0000 ~]$ wwall -j 28757187
Total CPU utilization: 0%
          Total Nodes: 1
                                                   Warewulf
               Living: 1
          Unavailable: 0
                                              Cluster Statistics
             Disabled: 0
                                         http://warewulf.lbl.gov/
                Error: 0
                 Dead: 0
                          CPU
                                    Memory (MB)
                                                     Swap (MB)
 Node
           Cluster
                                                                    Current
                       [util/num] [% used/total]
Name
            Name
                                                   [% used/total]
                                                                    Status
n0215.1r6
                        0%
                             (40) % 3473/192058
                                                   % 1655/8191
                                                                    READY
```

scancel <jobID> : cancels a job

More Information of **Slurm Usage**

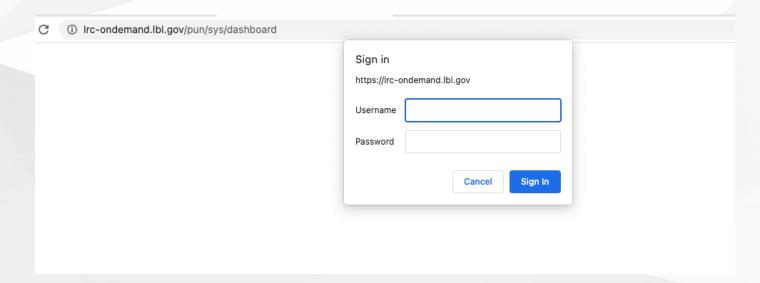
Open OnDemand (OOD)

- OpenOnDemand is a web platform that provides an easy access to the cluster's HPC resourses and services.
- Designed and developed by Ohio Supercomputer Center.
- Intuitive and easy access to computing resourses, alternative and convenient way to traditional command line access
- Allow access to Lawrencium compute resources
 - File browser: file editing, data transfer
 - Shell command line access terminal
 - Job monitoring
- Interactive applications: Jupyter Server, RStudio Server, MATLAB, Desktop
- Sever: https://lrc-ondemand.lbl.gov/
 - Intel Xeon Gold processor with 32 cores, 96 GB RAM

Accessing OOD on Lawrencium

1. Web link to connect: https://lrc-ondemand.lbl.gov/

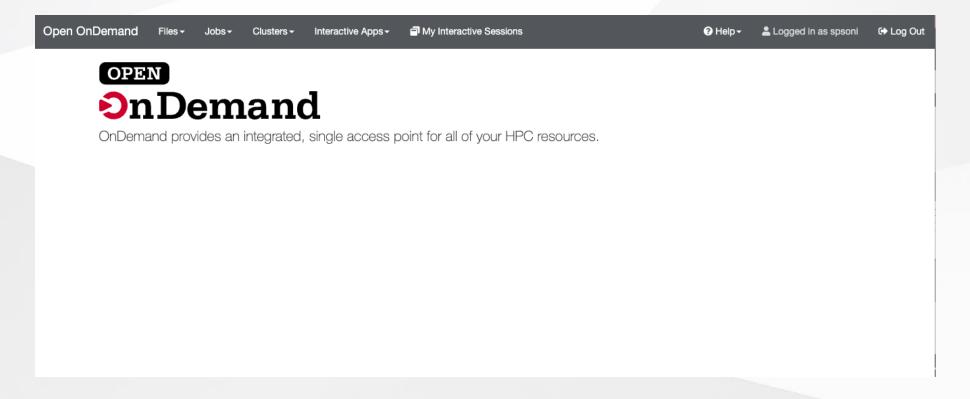
Note: Use Chrome or Firefox to browse this page. Safari has known <u>authentication issues</u>.



- 2. Use your LRC username and PIN+one-time password (OTP)
 - same credentials you use to login Lawrencium cluster

OOD Dashboard on Lawrencium

On successful authentication you will see a OOD dashboard.



Lets do quick demo!

Want to learn more about MyLRC portal? Join HPCS trainign on 7th February.

Getting help

- Virtual office hours:
 - Time: 10.30 am to noon every Wednesday
 - Online <u>request</u>
- Send us tickets at hpcshelp@lbl.gov
- More information about LBNL Supercluster and scientic computing services can be found here.
- Looking for more trainings? Upcoming training are regularly announced here. Other than LBNL HPC trainings you can also access DLab courses.

Submit FAQ here.

Your feedback is important to us for improving HPC services and training. Please fill out training survey

