PSC Bridges-2 Guide: Fall 2022 Edition

The Pittsburgh Supercomputing Cluster (PSC) provides powerful systems for high-performance computing to researchers and universities. It is located at 300 S Craig St, Pittsburgh, PA 15213.

In 15-418, we often use these machines for Assignments 3 and 4. You have the option to use them for your final projects as well.

For more information on what kind of resources the PSC provides, please see this page on their newest supercomputer, Bridges-2 (https://www.psc.edu/resources/bridges-2).

Creating Accounts for PSC

1. Create an ACCESS Account and specify tour ACCESS username in the Google Form posted on Piazza. https://piazza.com/class/l6dq8p7xw1j635/post/221
2. You should receive an email several hours later with a PSC username. These will be your credentials for SSH-ing to the PSC. Note that this may be different from your ACCESS username.

3. Visit the PSC Password Change Utility to select an initial PSC password. This will be used to SSH into the PSC machines.

Connecting to Bridges-2

Bridges-2 has login nodes which are used for managing files and submitting batch jobs, as well as compute nodes which perform intensive computations. When you connect to Bridges-2, you

are connecting to a login node, and may run interactive sessions or batch jobs on compute nodes as desired.

To connect to Bridges-2 over SSH: use your PSC username from the "Access to PSC" email from above. You will be prompted for your PSC password that you provided in the Password Change Utility.

```
$ ssh <psc_username>@bridges2.psc.edu
```

Compute Nodes

For 15-418, we have access to the Regular Memory (RM) and V100 GPU compute nodes. These nodes are further subdivided into shared and non-shared nodes:
- In **shared** nodes, users may choose to allocate only a fraction of the available CPU/GPU units for each job. For smaller workloads that do not require the resources of the entire machine, using shared nodes may allow your job to move faster through the queue.
- In **non-shared** nodes, users will be allocated the entirety of the CPU/GPU resources available to that node. Jobs running on an RM node will be allocated all 128 CPU cores, and jobs running on a GPU node will be allocated all 8 GPU cores.

More information on the technical specifications of these compute nodes is given in the section below.

Interactive Sessions

Interactive sessions are one of the two ways to perform computations on Bridges-2; the other way is to use batch jobs. In interactive sessions, you type commands into a shell and receive live output. To start a session, use

```
$ interact -options
```

Options	Description	Default
-p *partition*	Partition requested where `partition = RM	RM-shared	GPU	GPU-shared`	`RM-shared`
-t *HH:MM:SS*	Walltime requested (maximum 8 hours)	`60:00` (1 hour)
-N *n*	Number of nodes requested	1
--ntasks-per-node=*n*	Number of cores to allocate per node (Note: Only applies to shared partitions)	1
--gres=gpu:*type*:*n*	Number/type of GPUs requested where `n = 1-8` and `type = v100-16`	N/A

Do not run your code on the login server, as they are designed for submitting jobs and editing files. For intensive computations, you should start an interactive session first.

Batch Jobs

In batch jobs, you create a job script with commands to run and submit this job to a queue. The job will run as soon as resources are available, and on completion the command-line output will be written to a file called `slurm-`*`jobid`*`.out` in the same directory that the job was submitted from.

You may submit any script you'd like as a batch script, as long as the first line indicates what shell you are using (e.g. `#!/bin/bash`, `#!/usr/bin/python3`, etc.).

You can also manage your upcoming and completed jobs using the following commands:
- `squeue -u` *`username`*   Show jobs that belong to you on the queue
- `scancel` *`job_id`*   Cancel a specific job ID
- `job_info` *`job_id`*   Show information on completed jobs

To submit a batch job, use the following command:

`$ sbatch -`*`options`* *`script_filename`*

Options	Description	Default
`-p` *`partition`*	Partition requested where `partition = RM` `| RM-shared | GPU | GPU-shared`	RM
`-t` *`HH:MM:SS`*	Walltime requested (maximum 8 hours)	`30:00` (30 min)
`-N` *`n`*	Number of nodes requested	1
`--ntasks-per-node=`*`n`*	Number of cores to allocate per node (Note: Only applies to shared partitions)	1
`-o` *`filename`*	Name of output file (relative to the directory that the job was submitted from)	`slurm-`*`jobid`*`.out`
`--gpus=`*`type`*`:`*`n`*	Number/type of GPUs requested where `n = 1-8` and `type = v100-16`	N/A

Programming Environment (as of Fall 2022)
For Assignment 3, Bridges-2 automatically provides OpenMP support using the `-fopenmp` compiler flag. However, for Assignment 4, MPI must be separately loaded using the command shown below.

You can use the [module package](#) to load different versions of software that are not available by default. Here are some modules that may be useful:

- `module load openmpi/4.0.2-gcc8.3.1` For OpenMPI support
- `module load cuda` For CUDA support
- `module load nvhpc` For nvcc/nvc++
- `module load gcc/10.2.0` For an updated version of gcc
- `module load intel/2021.3.0` For icc/ispc

Here are some additional commands provided by the module package:

- `module avail` *package_name* See what modules are available for a software package
- `module load` *package_name* Load a given module (use `module unload` to unload)
- `module list` List all currently loaded modules
- `module purge` Unload all modules

Compute Node Technical Specifications

In 15-418, we are allocated 50,000 CPU core-hours on the regular memory nodes and 2,000 GPU unit-hours on the GPUs. Here are the technical specifications for each type of node:

1. **Regular Memory** (512x)
   - CPU: 2x AMD EPYC 7742 (2.25-3.40 GHz, 2x64 cores per node)
   - RAM: 256 GB
   - Cache: 256 MB L3 cache, 8 memory channels
   - Local Storage: 3.84 TB NVMe SSD
   - Network: Mellanox ConnectX-6-HDR Infiniband 200Gb/s Adapter
2. **V100 GPU** (9x)
   - GPU: 8x NVIDIA V100-16GB
   - CPU: 2x Intel Xeon Gold 6148 (2.40-3.70 GHz, 2x20 cores per node)
   - RAM: 192 GB, DDR4-2933
   - Interconnect: PCIe
   - Cache: 2.75 MB last level cache, 6 memory channels
   - Local Storage: 4x 2 TB NVMe SSD
   - Network: 2x Mellanox ConnectX-6-HDR Infiniband 200Gb/s Adapter

Note that we do not have access to the Extreme Memory (EM) or SXM2 GPU nodes, which are also provided by Bridges-2.

User Guide

For more information on PSC and Bridges-2, please see the [Bridges-2 User Guide](#)