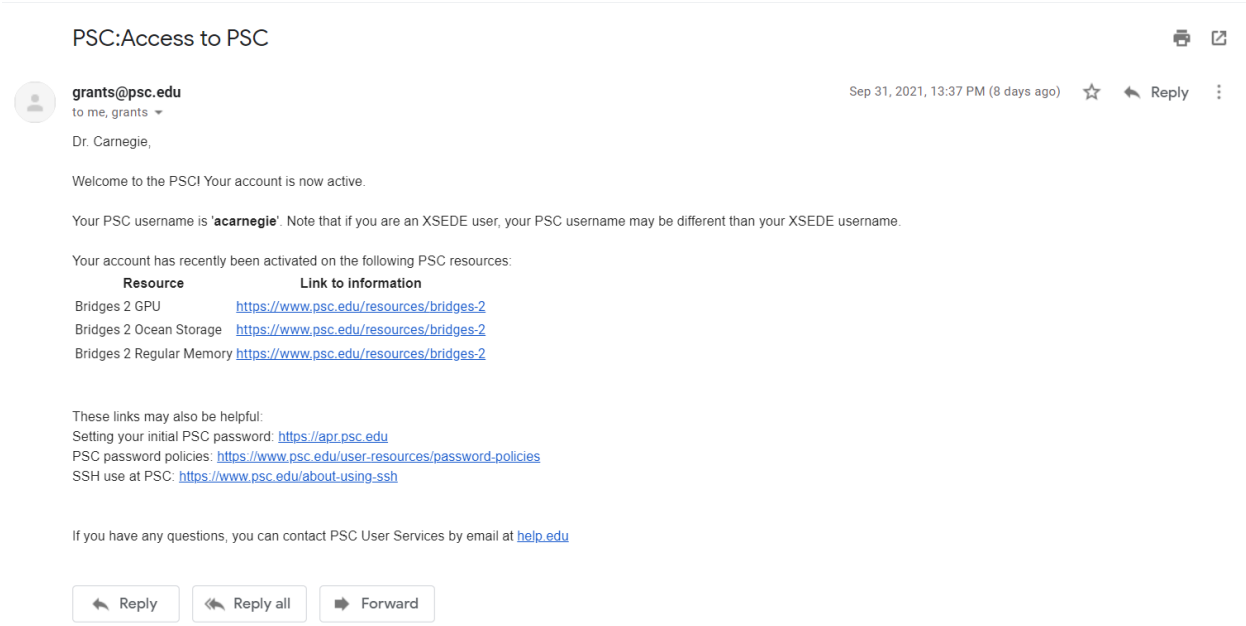
PSC Bridges-2 Guide

The Pittsburgh Supercomputing Cluster (PSC) provides powerful systems for high-performance computing to researchers and universities. In 15-418, we will be using 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 the PSC

1. Please visit the XSEDE User Portal and select **Create Account**. Once you do so, you will be asked for a verification code to verify your email.
2. In order to get added to the 15-418 organization, please specify your XSEDE username in the Google Form posted on Piazza.
3. 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 XSEDE username.



PSC:Access to PSC

grants@psc.edu
to me, grants

Sep 31, 2021, 13:37 PM (8 days ago) Reply

Dr. Carnegie,

Welcome to the PSC! Your account is now active.

Your PSC username is '**acarnegie**'. Note that if you are an XSEDE user, your PSC username may be different than your XSEDE username.

Your account has recently been activated on the following PSC resources:

Resource	Link to information
Bridges 2 GPU	https://www.psc.edu/resources/bridges-2
Bridges 2 Ocean Storage	https://www.psc.edu/resources/bridges-2
Bridges 2 Regular Memory	https://www.psc.edu/resources/bridges-2

These links may also be helpful:
Setting your initial PSC password: https://apr.psc.edu
PSC password policies: https://www.psc.edu/user-resources/password-policies
SSH use at PSC: https://www.psc.edu/about-using-ssh

If you have any questions, you can contact PSC User Services by email at help.edu

Reply Reply all Forward

4. Visit the PSC Password Change Utility to select an initial PSC password.

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 at Step 4.

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

If you prefer, you can also register SSH keys using your PSC username and password at this link: http://grants.psc.edu/cgi-bin/ssh/listKeys.pl

Compute Nodes
In 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.
    - For Assignment 3, you should use RM-shared nodes to run programs that only require one or two cores.
- 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.
    - For Assignment 3, you should use RM nodes to run your performance measurements.

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`*

Selected 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`

Selected 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 2021)

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 and the XSEDE User Portal