Faculty Guide to the Cal Poly Pomona

High Performance Computing (HPC) Cluster

Updated: 7-30-20

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2 INTRODUCTION

As part of its commitment to providing a state-of-the-art research and teaching environment to its faculty and students, Cal Poly Pomona operates a High Performance Computing (HPC) Cluster, managed by the campus Division of Information Technology & Institutional Planning. The new system entered production as a campus-wide resource in the Fall 2017 term and has been used to teach multiple courses in multiple disciplines. It is also currently being used as a resource for NSF-funded research and as a teaching resource in Cyber Security projects for Cal Poly Pomona undergraduates.

The new CPP HPC system is designed to serve researchers across campus. Initial research opportunities have already been identified within the Colleges of Science, Engineering, Business and CLASS and work is currently underway to integrate the HPC Cluster service into the campus Cyber Security Instructional Research Project (CSIRP), which serves as a resource hub for cross-disciplinary research in this growing field.

3 GETTING STARTED

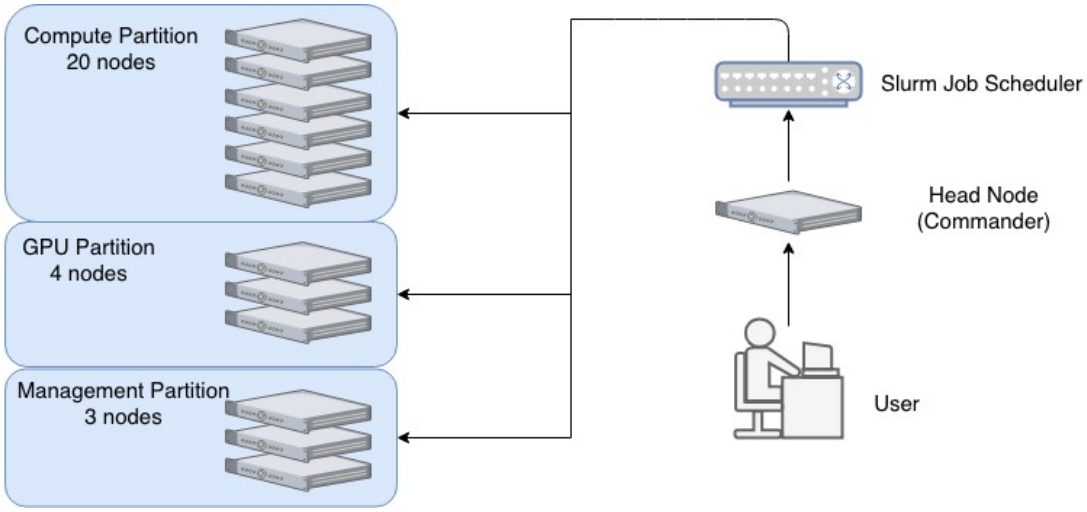
3.1 HARDWARE AND SPECIFICS

The High Performance Computing Cluster consists of multiple dedicated processor nodes, connected together via a specialized high-speed network and managed by specialized job scheduling software. The CPP HPC software management suite utilizes the HP Enterprises HPC Software Stack, which includes the open source Slurm job scheduler, Insight CMU for cluster Management, and other HPE software for node deployment and configuration. The system also has available the Anaconda package management system to allow users to install and manage their own dedicated libraries and external software packages.

The Slurm scheduler manages the allocation, dispatching and execution of jobs. Slurm is a popular and well documented package currently used by a large number of campus HPC systems and one that allows a task to be dispatched in a variety of ways, including allowing jobs to be run in real time, or in batch mode for longer running tasks.

The CPP HPC Cluster nodes are configured as a set of “partitions” to allow dispatching jobs to appropriate nodes for a variety of computational tasks. The “General Compute Partition” is used for general purpose jobs that benefit from running multiple compute tasks in parallel, while the “GPU Partition” allows a task to access dedicated GPU processors where the task would benefit from additional numerical processing capability.

The new CPP HPC cluster is based upon the HP Proliant server platform and currently includes a total of two DL360 management nodes, 20 DL160 compute nodes, and four GPU nodes with a total of 8 Tesla P100 GPUs The cluster contains 3.3TB of RAM and is connected through a dedicated internal 40GBit Infiniband switching fabric and 10 GBit external ethernet connections. The overall system throughput is currently approximately 36.6 Tflp in double precision mode or 149.6 Tflp in half precision mode. This current configuration is expected to grow over time, as researchers identify collaborative research initiatives and develop future funding for expansion of the system through external grants and donations.



3.2 GETTING STARTED AS A FACULTY MEMBER

3.2.1 Account Eligibility

The CPP HPC system is available to all faculty for either individual research or instructional use and to students either taking a course that requires access, or for individual faculty-supervised projects. Faculty may also request access for off-campus collaborators working on joint projects.

3.2.2 Applying for Faculty Account Access

To request activation of your individual faculty account, you may apply through the hpc-support web page:

https://www.cpp.edu/lrt/hpc/hpc-support.shtml

Alternatively, you may send an email to *HPC@cpp.edu* requesting that your faculty account be activated.

Once your request is received and your name added to the dedicated HPC Identity Management group you will be able to log in to the HPC control node using your campus BroncoName and associated password.

Note that access to the HPC cluster is through a Linux command line interface, so you will need to use a suitable terminal emulation program such as ssh or putty to initiate your connection. Additional details on logging in are provided in a later section of this guide.

3.2.3 Giving Your Students HPC Access

Faculty may request access for students in two ways, either through a sponsored student account for an individual student, or by requesting a course account for a specific course and/or section, which would provide access to all students registered for that class. To activate either type of account, begin by entering a request at the above hpc-support webpage with details of what you need (course number, term and any other special requirements). Staff will enable access for all students enrolled in the specified course for the duration of the term.

If the request is for an individual student, you will need to provide the student's name and associated BroncoName, as well as the details of the intended use (e.g. if the account is for a specific project, or to allow the student to participate in a specific faculty instructional research activity) and the anticipated duration of the access. By default, access is granted on a per semester basis, but longer can be provided, if needed.

3.2.4 Gaining Access for Off-Campus Collaborators

If you wish to work with collaborators from off campus, they will first have to apply for a campus "Affiliate" account, which will enable them to receive their own BroncoName and password. Once they have that, you may request access using the HPC support webpage, specifying nature of the intended work and duration required for the account. By default, initial quotas will be the same as for on-campus faculty accounts but can again be adjusted, if required.

Here is a link to campus Affiliate Account Application:

Here is a link to our HPC Support page:

3.3 User Quotas

3.3.1 Faculty File System Quotas

Each faculty member is initially assigned 25GB of file storage space in their home directory by default. If this is insufficient for your project needs, please let us know via the webpage and we can increase this amount.

Please Note: *Although there are file system quotas implemented on the user home directories, there are currently no quotas assigned in the new "data03" volume, but given its size and available resources, this partition is not currently being backed up so it should not be used for long term file storage. You may leave files there, but should take care to also ensure that additional copies are available to you either in your HPC home directory, or on another machine on the Internet.*

3.3.2 Student File System Quotas

Each student account is also currently being given 25GB of file storage space by default.

3.3.3 System GPU Quotas

Note: There are currently no Faculty quotas or limits implemented limiting access to the GPU partition but GPUs must be explicitly requested when a job is run with the slurm scheduler. By default, student jobs are restricted to 2 GPUs, access to more may be granted, if needed.

3.4 Provide Access to the Student Guide

Note that in addition to this HPC Faculty Handbook, there is a companion HPC Student Handbook available to help familiarize your students with the system. We recommend that you encourage your students to download the HPC Student Handbook.

3.5 A Note on the Landlord Tenant Model

The campus has funded a baseline deployment of resources to ensure that the system can be made available to all potential users but as demand for access to resources, the plan is to implement the conventional "landlord/tenant" model to control access to available resources. In this model, researchers who contribute hardware components to the system will have preferential access to their contributions, which are then made available to others on an "as-available" basis to other users.

4 FAMILIARIZING YOURSELF WITH THE TECHNOLOGY

4.1 LOGGING ON

To access and run jobs on the CPP HPC system, you must first log onto the system Command Partition using your CPP login credentials (BroncoName and associated password). To do this, you will need access to an ssh-enabled terminal emulation program, such as PuTTY on Windows, iterm2 for Mac or the Linux ssh command https://www.ssh.com/ssh/command.

When using the GUI-based tools, you will need to specify the hostname (“hpc.cpp.edu”), as well as the connection type (“SSH”) and port number (22). You should be prompted for your login name and password and once supplied, if you have Single Sign On enabled, you will be prompted for second factor authentication (e.g. a message to your phone). Once authentication is complete, you will be placed into the Command partition shell in your account home directory.

To do this on a Linux machine, type the following command:

ssh -l bronconame hpc.cpp.edu

NOTE: You must be connected directly to the campus network or be connected to the campus network via a virtual private network or VPN in order to access the HPC cluster.

For more information on how to connect to the campus VPN, please refer to this eHelp article on how to set up a VPN.

4.2 Familiarizing Yourself with the Command Line

Once logged on, you will find yourself in a traditional Linux command shell with the usual associated system commands, as well as access to the Anaconda package management system, the slurm job scheduler and other related tools. In this section, we provide a brief overview of the most common Linux commands, a brief summary of the Ananconda package management system and basic slurm command line options.

4.2.1 Common Linux Commands

The following Table summarizes some of the most common Linux commands you will need:

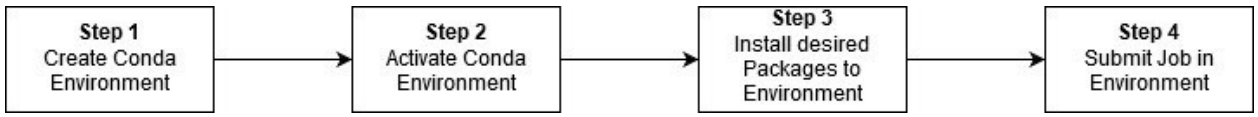
Useful Linux Commands		
Command	**Summary**	**Example**
cd path	Changes directory	cd project
ls	Lists all items in specific directory	ls
cat filename	Displays contents of a file	cat example.sh
touch newfilename	Creates a new file by that name	touch example
chmod filename	Changes the permissions of the file Options: (r, w, x) read write execute	chmod +x example.sh
time command	Written before any command, it outputs the time the command took. In the output, it will show three different times: - Real- wall clock time from start to finish - User- amount of CPU time spent executing the program - Sys - the amount of CPU time spent in the kernel	time hostname
man command	Shows the manual page for the command	man time

4.3 INTRODUCTION TO THE ANACONDA PACKAGE MANAGER

If you are developing a basic HPC program from scratch, you will likely need only a text editor and the common Linux command line options to create and manipulate your files, but if your work involves importing and configuring a system or package that has been developed elsewhere you will need access to a package management tool. Some programming languages allow you to import modules directly into your projects. In addition, HPC users have access to the Anaconda package management system, which is pre-installed on the Command Partition head node, which can be used to install multiple local libraries, as needed.

Many projects require providing access to specific versions of supporting packages and dependencies which could, if installed globally could potentially cause problems for other users due to mismatches between specific package versions. To avoid this problem, Anaconda allows you to import needed packages, as well as any needed dependencies, into your local file system, allowing you to run your project independently, when needed.

You will need to carry out the following steps to install a set of packages to your home directory:



The following Table summarizes the Commands needed to carry out these steps:

Anaconda Cheat Sheet	
Function	**Command**
Create Conda Environment	conda create -n environmentname Or, if you already know what package is needed to be installed, try: conda create –n environmentname packagename
List Conda Environments	conda env list
Activate Conda Environment	conda activate environmentname
Search for available packages to install	conda search packagename
Install package to environment	conda install packagename
Submit Job in Environment	Refer to “Running a Program” below
Deactivate Environment	conda deactivate

4.4 RUNNING A JOB WITH THE SLURM JOB SCHEDULER

The ***slurm*** job scheduler is used to control execution of your programs across multiple CPUs and GPUS. To execute a batch job utilizing one or more of the HPC compute or graphics nodes, you run slurm, telling it what cluster resources you need (such as type and number of nodes, number of individual tasks to allow at the same time, etc).

4.4.1 Common Slurm commands

Useful SLURM Commands		
Command	**Summary**	**Example**
srun -parameter job	Obtain a job allocation and execute an application (see Running a Program - SRUN)	srun -N1 -n1 example.py
sbatch -parameter batchscript	Submit a batch script for later execution (see Running a Program - SBATCH)	sbatch -o example.sh
sacct	Display accounting data Use -j jobid to see status of specific job	sacct -j 1576
sinfo	View the status of the cluster's nodes and partitions	sinfo
squeue	Displays information of jobs in queue	squeue

For more detailed summary of Slurm commands, visit:
https://www.cpp.edu/lrt/hpc/docs/hpc_slurm_command_summary.pdf

4.4.2 Running an Interactive Program with SRUN

There are two ways to run a program in the cluster: the command srun and the command sbatch.

Projects intended to run in interactive mode should proceed through the following steps:

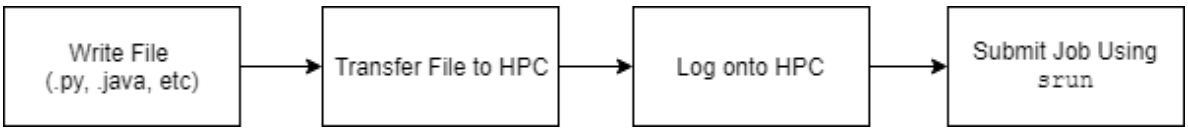


Diagram showing process of submitting a job through srun

Jobs submitted through the command srun are run interactively, which means that they run in the foreground rather than the background. Using the command srun allows you to run your project as a parallel job on the cluster managed by Slurm. It interrupts the command line to run the job, and the output goes directly to the command line unless an output file is specified.

As an example, type into your command line:

srun hostname

The node you are currently on is printed in the terminal. The head node, the one that you will begin on, is called commander.

To run a program you have written, the commands vary for different interpreters. To run a java program, first compile the .java file with:

srun javac filename.java.

Then to run the file enter:

srun java filename

Srun has many parameters that will be helpful and necessary when running your program. Below is a chart of different parameters that are often useful when using srun. For a more comprehensive manual on the different parameters and functions of srun, refer to:

https://slurm.schedmd.com/srun.html

With srun you can also set up an interactive session. To do this, type:

srun -N1 -n1 -p gpu --pty bash

This will begin an interactive session with one node in the gpu partition. You can run any number of commands within this shell. Once in the interactive session, you have direct access to the node. You can see the modules that the node has with the command:

module avail

This will show the resources that this particular node has.

Here is a list of useful commands that when navigating through the modules of a node:

module load - command adds application to your PATH variable pulling dependencies

module purge - removes all currently loaded modules module

unload - removes a specific module

module avail - browses entire list of modules

Useful Srun Parameters/Options		
Command	**Summary**	**Example**
-N#	Amount of nodes to be used for this job	-N1 Informs the head node to allocate 1 node for this job
-n#	Number of tasks in this job	-n1 Establishes that there is 1 task in this job
-p or --partition= partition name	Specific partition to be used for this job	-p compute Tells the head node to use the compute partition
--mem=<MB>	Memory to be allocated for this job	--mem=2GB
-o filename	Establishes a file to show the output	-o program.out
-w hostname	Tells Slurm to allocate a specified node	-w cn04
--test-only	Slurm will merely test your job and find out when your job is estimated to run, but does not actually submit job for execution	--test-only

4.4.3 Running a Batch Program with SBATCH

The command sbatch submits a batch script (it must be a batch script, not any other type) to Slurm that allocates the job a Job ID and submits it to be scheduled for later execution.

Projects intended to be run in batch mode should proceed through the following steps:

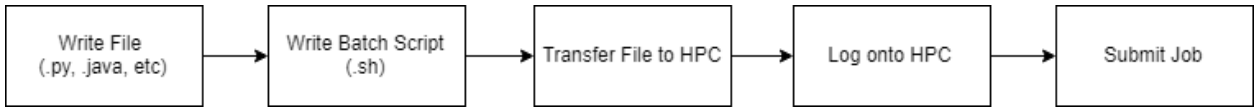


Diagram showing process of submitting a job through sbatch

Once the job is submitted, you will receive this message:

Submitted batch job jobid

You can see the queue at any time using the command squeue. To see the list of jobs you have submitted, use the command:

squeue --user bronconame

By default, the output is sent to a new file named slurm-jobid.ou. However, you can change this default by using the parameter -o filename. This will print the output onto the file specified instead of creating the default.

Since both srun and sbatch submit a job to SLURM for the schedule manager to run, the parameters for both commands are identical.

For more information about sbatch, the manual for the command can be found at:

https://slurm.schedmd.com/sbatch.html

4.4.4 Additional Information on Batch Scripts

A batch file is a text script that contains certain commands executed in sequence. Batch scripts enable the user to run multiple jobs in one command line. There are three parts to a batch script.

The first part is the program that will run the script. For a batch script, this is always:

#!/bin/bash

The second part of the batch script consists of directives for any jobs that are going to be called in the batch script. These directives tell Slurm the computational resources that the script requires. The directives use

#SBATCH -parameter

The final part is the actual script, consisting of commands to be run. Run jobs using srun as normal. You can reference other files and programs within the batch script to run.

Once the batch file is created, you must ensure that the user has permission to execute the script. To check the permissions of the file, use the command

chmod filename

To give the user permission to execute the file, use the command

chmod +x filename

The most commonly used directives for batch scripts are shown below:

Common Batch Script Directives		
Directive	**Description**	**Example**
--job-name=name or -J name	Custom job name	--job-name=example
--partition=name or -p partition	Partition to run on	--partition=compute
--nodes=# or -N#	Total number of nodes	--nodes=1
--ntasks=# or -n#	Number of "tasks". For use with distributed parallelism. See below.	--ntasks=1
--cpus-per-task=# or -c#	# of CPUs allocated to each task. For use with shared memory parallelism.	--cpus-per-task=1
--ntasks-per-node=#	Number of "tasks" per node. For use with distributed parallelism. See below.	--ntasks-per-node=2
--time=[[DD-]HH:]MM:SS or -t [[DD-]HH:]MM:SS	Maximum walltime of the job in Days-Hours:Minutes:Sec	--time=10:00 10 minutes
--mem=#	Memory requested per node in MB	--mem=1G

4.5 OTHER USEFUL TOOLS

4.5.1 Copying Files From Your Local Machine To the HPC

Using WinSCP or FileZilla

Log on with your bronconame and the cluster hostname: hpc.cpp.edu . Use the graphical interface to drag and drop files from local machine to the HPC. Alternatively, you may use your preferred FTP method.

NOTE: After copying a file, use command chmod +x filename to establish appropriate executable permissions

4.5.2 Available Languages and Resources

A variety of software is installed on the cluster for student and faculty use, including but not limited to:

Available Languages and Resources				
Python	Java	R	Keras	Pandas
Bioperl	Conda	Pycuda	Singularity	Tensorflow

In order to see which libraries are available on specific nodes, start an interactive session (see **Running a Program** for more information) and type:

module avail

4.6 POLICIES AND BEST PRACTICES

The following is an initial list of HPC best practices and pointers to appropriate CSU and CPP policies. These policies & best practices are subject to change. Please refer to the appropriate websites for updates.

4.6.1 HPC Best Practices

Users of the HPC are expected to adhere to the following set of "HPC Cluster Best Practices", which are intended to ensure stable and reliable operation of this shared resource.

1) The CPP HPC Cluster is a resource for academic research and instruction only.
2) Users are forbidden from accessing any data or programs for which they do not have specific authorization.
3) The HPC mass storage system is not intended for long term storage or backup of data. User data is not backed up to an external system and no data recovery services are available, so users are expected to make external copies of any data used or generated on the system.
4) Users are also expected to delete data or programs from the HPC cluster once it is no longer needed.
5) Users are requested to acknowledge the use of the HPC cluster in their research publications. A sample acknowledgement is as follows:

4.6.2 CSU System-wide IT and IT Security Policies

Users of computer systems within the CSU system are required to follow system-wide IT and IT Security policies. The most recent versions of these policies may be found at:

https://calstate.policystat.com/

This is a searchable page of all CSU-wide policies. To start, enter keyword "Information" to see an initial list of IT and IT Security related systemwide policies.

4.6.3 Cal Poly Pomona IT and IT Security Policies

In addition to the CSU system-wide policies, Cal Poly Pomona currently has campus-specific IT policies covering Appropriate Use of IT devices and use of the Web for publishing. These may be found at:

https://www.cpp.edu/policies/university/information-technology/index.shtml

4.7 ACKNOWLEDGEMENTS

Users are requested to acknowledge the use of the HPC cluster in their research publications.

A sample acknowledgement is as follows:

> *"This work used the High Performance Computing Cluster and the Mass Storage System at California State Polytechnic University, Pomona, which was supported in part by the university and NSF grant MRI-1828644."*

4.8 HPC QUESTIONS AND SUPPORT

You are now ready to get started with the Cal Poly Pomona HPC system. If you have any additional questions please feel free to contact the support team by sending email to the HPC@cpp.edu email address. Additional assistance may be acquired through our HPC support form.

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