GETTING STARTED ON THE VACC

Vermont Advanced Computing Center

Shelly Johnson

Senior Research Computing Facilitator

Bennet Fauber

Senior Research Computing Systems Engineer

High Performance Computing

- A High Performance Computing (HPC) cluster is a collection of many computes networked together

- Each computer is called a node.

- HPC clusters run computations managed by a scheduler p...

- The scheduler keeps track of available resources, allowing requests to be efficiently assigned to compute resources
  - memory, processing power (cpu or gpu), time, or some combinat...

Node Types

Login Node

When you log onto a cluster you land on a login node.   Edit scripts, run short tests, and
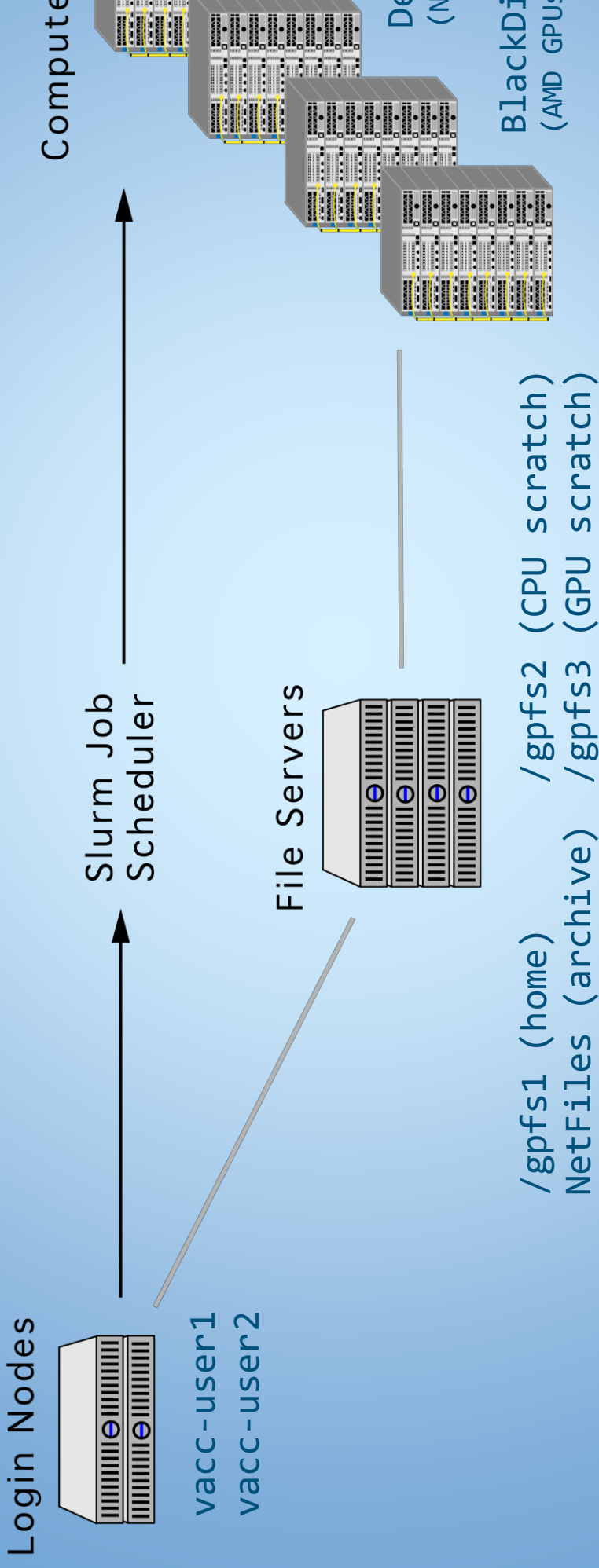
`[ <netID>@vacc-user1 ~] $`

Rough guidelines: the test will run < 5 minutes, use less than 8-12 GB of memory, and u (less is better)

If more resources are needed, use a regular job or an interactive job or Open OnDeman

Compute Node

Compute nodes are where all the heavy lifting is done. Once on a login node, you can s jobs either in batch form or interactively to the compute nodes.

The VACC Cluster

Compute

Login Nodes
vacc-user1
vacc-user2

Slurm Job Scheduler

File Servers

/gpfs1 (home)
NetFiles (archive)

/gpfs2 (CPU scratch)
/gpfs3 (GPU scratch)

BlackDi
(AMD GPUs

De
(N

Slurm

All jobs are run on the compute nodes using the Slurm Workload M

Slurm needs to have the following information about what you wan

○ The partition (group of nodes) to use

○ Number of CPUs

○ Amount of memory

○ Amount of time needed to run

○ Whether you need a GPU, and if so, how many

These are the boxes you will fill in when starting a job

For further information about Slurm, see the User Guide

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

Modules on VACC

- Modules are used to modify your environment to access software p
  installed on the cluster

- Modules can be loaded on the command line or in your batch scrip

  ○ It is preferred to load them in your batch script to have a record of which module
  loaded if there is a problem with your job

Load Software on VACC: MODULES

Show which modules are available:

```
$ module av
```

Load a module and list the loaded modules (including depend

```
$ module load Rtidyverse/4.3.2
$ module load rstudio
$ module list
```

Unload modules:

```
$ module unload Rtidyverse rstudio
$ module purge
```

Load Software on VACC: Spack

Show which packages are available:

```
$ spack find
```

Load a package and list the loaded software (including depe

```
$ spack load bowtie@1.2.3
$ spack find --loaded
```

Unload a Spack package:

```
$ spack unload bowtie
```

Open OnDemand (OOD)

- Submit jobs via a web interface: https://vacc-ondemand.uvm.edu

- Choose between a Desktop or any of the following apps:
  - Jupyter Notebook
  - Rstudio
  - MATLAB* (coming soon)

Guide to using the VACC Open OnDemand

https://www.uvm.edu/vacc/kb/knowledge-base/ondemand/

```
#!/bin/bash
#SBATCH --job-name=example
#SBATCH --time=00:15:00
#SBATCH --ntasks=2
#SBATCH --mem=8G
#SBATCH --nodes=1
#SBATCH --account=<account
#SBATCH --partition=bluemo
#SBATCH --mail-user=<netI
#SBATCH --mail-type=BEGIN

module purge
module load python3.11-ana
module list

python my_python_script.py
```

- A batch script is the script used to submit a job to the cluster. Batch scripts end with either *.sbat* or *.sh*

- The example shown is a simple batch script that loads a Python module and runs a Python script.

- Modules should be loaded after the #SBATCH lines and before any commands

Submitting a Job to the Cluster

Check your that your script specifies all required resources, the accoun
partition are accurate, and all of your modules loaded

To submit your job to the cluster

```
$ sbatch <script_name>.sbat  (or .sh)
```

Check the status of your job

```
$ squeue -u <user>
```

```
JOBID  PARTITION    NAME      USER   ST  TIME  NODES  NODELIST(REASON)
325511  bluemoon   testjob  mjohns89   R  0:00    1   node200
```

Helpful Commands

```
my_accounts                    : list your cluster accounts
my_job_statistics <jobID>      : show resources used for a comp
squeue -u <user>               : check all jobs for a specific u
scancel <jobID>                : cancel a job
```

Resources

VACC Knowledge Base: https://vacckb.helpline.w3.uvm.edu/vacc/kb/

Open OnDemand (web interface): https://vacc-ondemand.uvm.edu/

Open a support ticket: vacchelp@uvm.edu