Getting started on Prince

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Logging in to Prince

Logging in to Prince is the same 2-stage process as logging into any other NYU HPC cluster. The host name is 'prince.hpc.nyu.edu'. The HPC cluster Prince is not directly visible to the internet (outside the NYU Network). If you are outside NYU's Network (off-campus) you must first login to a bastion host named hpc2.nyu.edu.

NOTE: The clusters can still access the internet directly. This may be useful when copying data from servers outside the NYU Network - see: How to copy files to and from the HPC clusters.

NOTE: Alternatively, instead of login to the bastion host, you can use VPN to get inside NYU's network and access the HPC clusters directly. Instructions on how to install and use the VPN client are available here.

NOTE: You can't do anything on the bastion host, except ssh to the HPC clusters.

Adding Prince to your SSH Tunnel

On a Mac:
Files and directories on Prince

Mountpoint | Storage Capacity | FS Type | Backed up? | Flushed? | Availability | Variable | Value
---|---|---|---|---|---|---|---
/home | 43 TB (20 GB / user) | ZFS | Yes | No | All Prince nodes (login, compute) | $HOME | /home/$USER
/scratch | 1.1 PB (5 TB / user) | Lustre | NO | YES | Files unused for 60 days are deleted | All Prince nodes (login, compute) | $SCRATCH | /scratch/$USER
/beegfs | 500TB (2 TB / user) | BeeGFS | NO | TBD | All Prince nodes (login, compute) | $BEEGFS | /beegfs/$USER
/archive | 700 TB (2 TB / user) | ZFS | Yes | No | Only the login nodes | $ARCHIVE | /archive/$USER
/state/partition1 | Varies, mostly >100GB | ext3 | NO | YES | Separate local filesystem on each compute node | $SLURM_JOBTMP | /state/partition1/$SLURM_JOBID

Transferring files to Prince

Your files on /scratch are visible on Prince, and will remain such.

Moving many small files takes significantly longer than moving one large file. Therefore, to transfer source code with many small files from /home on another cluster, we recommend tarring up the source directory first.

We recommend rebuilding all models on Prince - this will ensure the best performance and also avoid any problems relating to mismatched OS and library versions between the clusters. Therefore, there is no need to transfer object files or executables.

How to migrate from another cluster to Prince
If you have a workflow on a previous cluster, and you wish to replicate it on Prince:

1. Ensure the files you need are available on Prince
   Files on \texttt{SCRATCH} are already available on Prince - there is nothing you need to do with these.
2. You will need to rewrite your scripts to convert them from using PBS to using Slurm Job Scheduler. If you are having any questions or issues, contact us for help.
3. Check your \texttt{.bashrc} and \texttt{.bash_profile} files. If on the older cluster, you loaded certain modules in them, you may wish to add corresponding lines to those files on Prince. You may also wish to replicate your shell aliases.
4. If you are running a model you compiled yourself, you will probably get improved performance by recompiling the model on Prince. See below for more about compiling code.

### Compiling Code on Prince

We recommend using the Intel compiler suite (\texttt{module load intel}), and, for MPI programs, OpenMPI (\texttt{module load openmpi/intel}).

The GNU compiler suite is also available (\texttt{module load gcc}) and over time other compiler versions and MPI implementations will be installed. There will be instances in which an alternative compiler or MPI library performs better or avoids a bug in the recommended compilers, but in the long run the functionality and performance of compilers and MPI libraries is very similar, so for easiest maintenance, only use the alternatives if you really need to.

If you are building software to use for many or long-running jobs, testing for performance with a few MPI libraries and compile options can be very valuable since a specific model might run noticeably faster under one MPI implementation than another.

### Submitting batch jobs on Prince

Prince cluster uses Slurm Job Scheduler, a resource manager designed to allocate compute resources and schedule jobs. Due to the nature of HPC clusters we recommend writing a batch script, rather than running interactive commands.

There are two aspects to a batch job script:

- A set of \texttt{SBATCH} directives describing the resources required and other information about the job
- The script itself, comprised of commands to setup and perform the computations without additional user interaction

Jobs are submitted with the \texttt{sbatch} command:

$ sbatch \texttt{options \texttt{job-script}}

The options tell SLURM information about the job, such as what resources will be needed. These can be specified in the job-script as \texttt{SBATCH} directives, or on the command line as options, or both (in which case the command line options take precedence should the two contradict each other). For each option there is a corresponding \texttt{SBATCH} directive with the syntax: \texttt{#SBATCH option} You can find a list of sbatch options here.

### Interactive sessions

To start an interactive batch session, use:

$ srun --pty /bin/bash

If you need a GUI, you should use:
By default single CPU core and 2GB memory are allocated to your job for 1 hour. You can explicitly request more CPUs and more memory with the following options:

```
$ srun --x11 --pty /bin/bash
```

The above command requests 4 compute nodes for 2 hours with 4Gb of memory.

Most nodes have either 64GB, 128GB, 192GB or 256GB of memory. However, some amount of memory is also needed by the operating system, so nodes have about 62GB, 124GB, 189GB and 250GB available for jobs. If you request 128GB, you restrict the job to the subset of nodes having more than 128GB of memory, and it will probably take longer to schedule.

### GPU Jobs

In Prince cluster, there are currently 9 GPU nodes. Each of the nodes is equipped with 4 Tesla K80 cards.

<table>
<thead>
<tr>
<th>GPU Name</th>
<th>Persistence-M</th>
<th>Bus-Id</th>
<th>Disp.A</th>
<th>Volatile Uncorr. ECC</th>
<th>Memory-Usage</th>
<th>GPU-Util</th>
<th>Compute M.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tesla K80</td>
<td>On</td>
<td>0000:04:00.0</td>
<td>Off</td>
<td>0%</td>
<td>0MiB / 11439MiB</td>
<td>0%</td>
<td>E. Process</td>
</tr>
<tr>
<td>N/A</td>
<td>22C</td>
<td>P8</td>
<td>26W / 149W</td>
<td>0%</td>
<td>0MiB / 11439MiB</td>
<td>0%</td>
<td>E. Process</td>
</tr>
<tr>
<td>Tesla K80</td>
<td>On</td>
<td>0000:05:00.0</td>
<td>Off</td>
<td>0%</td>
<td>0MiB / 11439MiB</td>
<td>0%</td>
<td>E. Process</td>
</tr>
<tr>
<td>N/A</td>
<td>28C</td>
<td>P8</td>
<td>30W / 149W</td>
<td>0%</td>
<td>0MiB / 11439MiB</td>
<td>0%</td>
<td>E. Process</td>
</tr>
<tr>
<td>Tesla K80</td>
<td>On</td>
<td>0000:06:00.0</td>
<td>Off</td>
<td>0%</td>
<td>0MiB / 11439MiB</td>
<td>0%</td>
<td>E. Process</td>
</tr>
<tr>
<td>N/A</td>
<td>20C</td>
<td>P8</td>
<td>26W / 149W</td>
<td>0%</td>
<td>0MiB / 11439MiB</td>
<td>0%</td>
<td>E. Process</td>
</tr>
<tr>
<td>Tesla K80</td>
<td>On</td>
<td>0000:07:00.0</td>
<td>Off</td>
<td>0%</td>
<td>0MiB / 11439MiB</td>
<td>0%</td>
<td>E. Process</td>
</tr>
<tr>
<td>N/A</td>
<td>29C</td>
<td>P8</td>
<td>30W / 149W</td>
<td>0%</td>
<td>0MiB / 11439MiB</td>
<td>0%</td>
<td>E. Process</td>
</tr>
</tbody>
</table>

To request one GPU card, use the Slurm directive:

```
#SBATCH --partition=gpu
#SBATCH --gres=gpu:1
```

### Software on Prince

Prince uses the same Environment Modules setup as previous clusters. Please check the availability of the module you need with:

```
$ module avail
```

Different versions of software may give slightly different results, especially if your model is numerically sensitive! Please carefully check the results of simulations on Prince and compare them to results on the cluster you used previously!