<table>
<thead>
<tr>
<th>Quick Links</th>
</tr>
</thead>
<tbody>
<tr>
<td>HPC Home</td>
</tr>
<tr>
<td>Getting an account</td>
</tr>
<tr>
<td>Getting started on Prince</td>
</tr>
<tr>
<td>Prince How-to Articles</td>
</tr>
<tr>
<td>Logging in</td>
</tr>
<tr>
<td>Windows</td>
</tr>
<tr>
<td>Mac / Linux</td>
</tr>
<tr>
<td>Clusters and Storage</td>
</tr>
<tr>
<td>Prince (HPC)</td>
</tr>
<tr>
<td>Dumbo (Hadoop)</td>
</tr>
<tr>
<td>Dalmatia (NYU Abu Dhabi)</td>
</tr>
<tr>
<td>Transfering data to/from the clusters</td>
</tr>
</tbody>
</table>
Transferri
ng data
to/from
Prince
cluster
using
Globus
Submittin
g jobs
with
sbatch
Available
software
Licensed
Software
Available
on the
HPC
Cluster
Building
Software
Slurm
Tutorial
Tutorials
FAQs
Scratch
Area
Cleanup
Programming for
Biologist
s
Acknowle
dge
Statement
Research
Gallery
HPC
People
HPC
Policies
Something went wrong!

Why does running "ls" on /scratch take so long?

I can't login

When trying to login, I get warning s about “HOST IDENTIFICATION HAS CHANGED”

What happened to my data on /scratch?

In the library, my wireless connecti on keeps dropping out. How can I fix it?

I'm getting a "module : command not found" error
Warning: no access to tty (Bad file descriptor), Thus no job control in this shell

I get an error "Warning: no display specified." when I use -X flag with ssh

Who killed my job, and why?

I got an email "Please do not run jobs on login nodes"

Running jobs

What resources can and should I request?

Can I make sure a job gets executed only after another one completes?

How do I log in to a specific node?

How can I make sure my job is running smoothly?
My job will take longer than 48 hours, what should I do?

My job needs (MySQL, some other service) to be running

I want to run a job at 9am every day

Using software

How do I run ...
(esp, needs a license)

a S T A T A job?

a G aussian job?

a M a job?
a parallel Non MPI job (e.g. Julia)?

I can't find (some software package)

Can you install (some software package)?

How can I view a PDF file on Prince?

Managing data

How much of my file/space quota have I used?

How do I give my colleague access to my files?

How do I get the best transfer speed to or from BuTinah?
Where am I?

How can I show the cluster name in the command prompt?

The login nodes of each cluster have names like "login-0-1". You can add the following idiom to your $HOME/.bashrc file to set the prompt to the name of the cluster:

```
# what cluster am I on?
CLUSTERNAME=NYU-HPC
ip=$(host $(hostname))
[[ $ip =~ 10.0.254.[0-9]+$ ]] && CLUSTERNAME=Prince
[[ $ip =~ 10.0.255.[0-9]+$ ]] && CLUSTERNAME=Dumbo
PS1='["$CLUSTERNAME": \u@\h \W]\$ ' 
```

Something went wrong!

My account expired! What should I do? Is my data gone forever?

You can renew your account even after it has expired, see Getting or renewing an HPC account for how to renew. Data on /home, /archive and /work is deleted 90 days after account expiration. Data on /scratch is deleted after 60 days of not being used, whether your account is current or expired.

Why is "ls" on /scratch so slow?

Lustre stores the file itself and the file metadata (its name, size, etc) separately. When you issue a simple 'ls' command, a remote procedure call (RPC) is made to the metadata server (MDS), which returns a list of the files in the current directory. If you add certain options, such as -l or --color=tty, then for each file in the list, ls will call stat() on that file. The stat() call involves an RPC to the MDS and an RPC to the object storage server (OSS) which holds the file itself. These RPCs, especially those to the OSS, can take a long time.

I can't login

I get a message about bad permissions

SSH is fussy about permissions on the $HOME/.ssh directory. It should have:

```
[ab123@myworkstation ~]$ ls -la $HOME
total 545460
drwx------  11 ab123 users 4096 Sep  4 11:19 .
drwxr-xr-x  3 root root 0 Aug 28 14:44 ..
drwx------  2 ab123 users 4096 Aug  8 11:19 .ssh
```

Note that .ssh has rw permission for the owner, and no permission at all for anyone else. You can set these permissions with the command:

```
[ab123@myworkstation ~]$ chmod 700 $HOME/.ssh
```
When trying to login, I get warnings about "HOST IDENTIFICATION HAS CHANGED"

Recent versions of OSX and Ubuntu have a newer version of ssh than the NYU HPC clusters. You can prevent the warnings with two steps:
1. Update .ssh/config on your workstation according to the example here.
2. Delete your .ssh/known_hosts fileYou will then be asked about connecting to a new host on the first time, you can safely answer "yes"

What happened to my data on /scratch?
The /scratch filesystem is a short-term filesystem providing fast I/O for running jobs. It is not backed up, moreover files which remain unused for a period of time a flushed. See Storage July 2017 - especially /scratch policy for further information.

Q: In the library, my wireless connection keeps dropping out. How can I fix it?
A1: If you are using a Mac:

OSX roams "aggressively", which means that if it can see multiple access points it will abandon a working connection to pursue another one which might be better. The Bobst library supports a lot of wireless users and thus has many wireless access points, and Mac laptops behave like an undisciplined child in a candy store, authenticating to one point only to then disconnect and try another. Some actions which might help:

- Under Network preferences->WiFi->Advanced, remove all NYU networks except "nyu" from the "preferred networks" list, and move "nyu" to the top of the list
- If that fails, you can disable the aggressive roaming from the terminal, with the command:

  sudo defaults write /Library/Preferences/com.apple.airport.opproam disabled -bool true

A2: If you are using Windows:

- If you are running the PeerGuardian personal firewall software, switch it off (it disables DHCP). Otherwise:

Recent versions of Windows take a supposedly-more-secure but also less reliable approach to authenticating to a wireless network, which causes network connections to be dropped unnecessarily. A pop-up bubble in the bottom corner of the screen which says "please re-enter your password" is an indication that this is happening.

- Instead of using the Windows-supplied wifi drivers, download and install the most recent driver from the manufacturer of your wireless-network-interface card

A3: if all this fails:
Come see the DS helpers - they may have another trick or two up their sleeve

Q: I used "module load" and it failed with a "module: command not found" error

Normally the location of the module command is set up when the shell is started, but under some circumstances that startup procedure can be bypassed. If you get this error you can explicitly prepare your environment for modules with one of the following commands:

- If your script (or interactive environment) uses bash (the default) or sh or ksh:

  source /etc/profile.d/env-modules.sh

- If your script (or interactive environment) uses csh or tcsh:

  source /etc/profile.d/env-modules.csh

In the case of a PBS job script, add one of the above lines before the first "module" command in your script.

If you are seeing the error in an interactive shell, run one of the above commands at the prompt, then attempt the "module load" command again.

Warning: no access to tty (Bad file descriptor), Thus no job control in this shell

It's harmless and does not indicate an error. This is an innocuous warning that simply means you are running a script (rather than a binary) under a job that has no access to the TTY. In other words, you cannot interrupt it (^C), suspend it (^Z) or use other interactive commands because there is no screen or keyboard to interact with it. It can be safely ignored.
Preparing your Mac for X

If you wish to use any software with a graphical interface, you will need an X server. This is a software package that draws on your local screen windows created on a remote computer (such as an NYU HPC cluster).

- Download and install XQuartz

Preparing your Windows workstation for X

If you wish to use any software with a graphical interface, you will need an X server. This is a software package that draws on your local screen windows created on a remote computer (such as an NYU HPC cluster). There are a couple of options out there:

- We recommend Cygwin/X. Instructions for downloading and installing it can be found here.
  Before starting PuTTY you will need to have the X server running, by double-clicking the "XWin Server" shortcut under Cygwin-X on the Start Menu. You may wish to add this to your Windows Startup folder so it runs automatically after starting Windows

- Another good option is Xming. Installation instructions can be found on its web site.
  As per Cygwin/X, you will need to launch Xming before starting PuTTY.

You will also need to download and install PuTTY SSH if you have not already.

Who killed my job, and why?

The most likely culprit is the batch system. The other prime suspect is us, the HPC system administrators. If the batch system killed your job, it probably did so because it exceeded the amount of memory or CPU time requested (which may have been some default, if you did not explicitly request these). See Submitting a job - Resource limits for help on this, and this overview of scheduling for a more general introduction.

If we killed your job, it was probably to prevent the system from crashing, which can happen when a jobs runtime behavior puts a certain type of load on the system. The most common trouble is non-optimal use of the /scratch filesystem, described at the bottom of the table on the Storage page. The next most common reason is that you were running your job on the login node rather than through the batch system - see Running jobs - Nodes for more on this. There are a few circumstances where the login node is the only option - especially archiving files to your $ARCHIVE directory - if you experience trouble with this please contact us. The /scratch filesystem is configured for large-block I/O, such as sequential reading and writing of large files. However individual I/O operations are relatively costly, so programs using frequent, small I/O accesses will put a heavy load on the metadata servers, which in extreme cases can cause the system to become unstable. The system administrators generally detect this quickly and may kill a job whose I/O characteristics are are stretching the capabilities of the filesystem (if this happens, we will contact you to help configure your job for better stability and performance).

I got an email "Please do not run jobs on login nodes"

The login nodes are a shared resource intended for editing scripts, compiling small amounts of code and moving data about. This is enforced via process size limits - if a command on a login node runs for too long or uses too much memory, the system will kill it and send you this email. The likely causes are:

- You are trying to run a simulation interactively instead of via the batch system. Please read Running jobs on the NYU HPC clusters, especially Writing and submitting a job for how to do this. If you need interactive use, read Submitting a job - Working interactively
- You are running a command on the login node that takes longer or needs more memory than you expected. Common causes include:
  - Opening a large (more than 1GB) file with Vim (try using "less" instead)
  - Compiling a large and complex source file
  - Compressing a large file with gzip

In most cases the best solution is to start an interactive session on a compute node, requesting sufficient resource for the task at hand - see Submitting a job - Working interactively

Running Jobs

What resources can and should I request?

For further details, see Submitting a job - Resource limits

Can I make sure a job gets executed only after another one completes?

A: Yes

This page is retained from an earlier version of the HPC wiki only for reference.
Where did my job output go?

How do I use GPUs?

How do I log in to a specific node?

A1: You can ssh to a specific login node. The login nodes on bowery are named login-0-0, login-0-1, login-0-2, login-0-3.

```bash
$ ssh login-0-0
```

A2: You can ssh to a specific compute node if you have a job running on it. To find out which nodes your job is running on use:

```bash
$ qstat -n
```

You will see the usual qstat output followed by a list of the nodes and cores your job is allocated to. The list will look something like:

```
In this example, the list shows cores 11 and 10 on node compute-6-3.
```

How can I ensure my resource-intensive job is running smoothly?

A: After submitting jobs, you will be able to locate where your jobs are executing by running `pbstop -u NetID`. Then you can monitor these jobs by logging in to the corresponding compute nodes and running `top`. You will then see both CPU and memory consumptions. If you find little memory left (or even little swap left) due to your job, you should increase the "ppn" number in your PBS script or maybe consider taking advantage of the nodes with larger memory

(more...)

My job will take longer than 48 hours, what should I do?

For long-running jobs, we suggest using `Checkpoint-Restart` to split the job into a series of shorter jobs. We realize though that this is not always possible - if you need the walltime limit for a job extended, contact us.

My job needs (MySQL, some other service) to be running

Contact us.

I want to run a job at 9am every day

(still to come)

Using Software

There are usage examples for many popular software packages in `/share/apps/examples` on Prince:

- `batch` - An example batch job
- `blcr` - Checkpoint-Restart facility for long jobs
- `comsol` - Computational Fluid Dynamics
- `c-sharp` - Language for the .NET/mono runtime environment
- `fluent` - Computational Fluid Dynamics / Multiphysics package
- `gaussian` - Chemistry package
- `matlab` - For mathematical exploration
- `namd` - Molecular dynamics
- `qchem-amber` - Molecular dynamics
- `r` - Interpreted language for statistics work
- `resource-usage` - Shows minute-by-minute CPU and memory usage of a program
- `stata` - Statistics package

How do I run a STATA job?

(more...)

How do I run a Gaussian job?

(more...)

How do I run a Matlab job?

(more...)

How do I run a R job?
Basic R jobs

Multiple R versions exist in HPC environment. To check what are available, on Prince:

```
$ module avail r
```

<table>
<thead>
<tr>
<th>Module Name</th>
<th>Version</th>
</tr>
</thead>
<tbody>
<tr>
<td>r/intel/3.0.3</td>
<td>ray/openmpi/intel/20160114</td>
</tr>
<tr>
<td>reprozip/intel/1.0.3</td>
<td>rpy2/intel/2.5.6</td>
</tr>
<tr>
<td>r/intel/3.1.2</td>
<td>rdkit/intel/201409.2</td>
</tr>
<tr>
<td>requests/2.7.0</td>
<td>rseqc/intel/2.3.9</td>
</tr>
<tr>
<td>r/intel/3.2.0</td>
<td>recon/intel/1.08</td>
</tr>
<tr>
<td>ribopicker/0.4.3</td>
<td>rseqc/intel/2.3.9</td>
</tr>
<tr>
<td>r/intel/3.2.2</td>
<td>rdp_classifier/2.11</td>
</tr>
<tr>
<td>rmblast/2.2.28</td>
<td>rstudio/0.98.1028</td>
</tr>
<tr>
<td>randfold/intel/2.0</td>
<td>ray/openmpi/intel/20160114</td>
</tr>
<tr>
<td>rose/20151118</td>
<td>rendertoolbox3/2.1-18</td>
</tr>
<tr>
<td>raxml/intel/7.3.0</td>
<td>repeat_masker/4.0.5</td>
</tr>
<tr>
<td>rosetta/intel/54167</td>
<td>repeatmodeler/1.0.8</td>
</tr>
<tr>
<td>raxml/intel/8.0.23</td>
<td>rosetta/openmpi/intel/2014.35.57232</td>
</tr>
<tr>
<td>rosetta/intel/8.2.5</td>
<td>repeatmodeler/1.0.8</td>
</tr>
<tr>
<td>rosetta/openmpi/intel/2014.35.57232</td>
<td>repeatscout/intel/1.0.5</td>
</tr>
<tr>
<td>rosetta/openmpi/intel/54167</td>
<td></td>
</tr>
</tbody>
</table>

Suppose we want to use 3.3.2, run these commands:

```
$ module purge
$ module list
No Modulefiles Currently Loaded.
$ module load r/intel/3.3.2
$ module list
```

```
Currently Loaded Modulefiles:
1) intel/14.0.2          4) cairo/gnu/1.12.16          7) mpfr/gnu/3.1.2          10)
2) zlib/intel/1.2.8      5) expat/intel/2.1.0         8) mpc/gnu/1.0.2          11)
3) bzip2/intel/1.0.6     6) gmp/gnu/5.1.3            9) gcc/4.8.2        12)
13) openssl/gnu/1.0.1g   14) curl/intel/7.38.0   15) openmpi/intel/1.6.5
```

```
$ R
```

We first clean up the environment by doing ‘module purge’. Then we load the R version selected, check what are available in current environment. We can see that R 3.3.2 is indeed loaded along with its dependency modules. Let's try this basic R example. We name it “example.R”:

```
df <- data.frame(x=c(1,2,3,1), y=c(7,19,2,2))
df
indices <- order(df$x)
order(df$x)
df[indices,]
df[rev(order(df$y)),]
```

Below is the screen scene while running it on Prince:
$ R

R version 3.3.2 (2016-10-31) -- "Sincere Pumpkin Patch"
Copyright (C) 2016 The R Foundation for Statistical Computing
Platform: x86_64-centos-linux-gnu (64-bit)
R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.
Natural language support but running in an English locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.
Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> df <- data.frame(x=c(1,2,3,1), y=c(7,19,2,2))
> df
   x y
1 1 7
2 2 19
3 3 2
4 1 2
> indices <- order(df$x)
> order(df$x)
[1] 1 4 2 3
> df[indices,]
   x y
1 1 7
4 1 2
2 2 19
3 3 2
> df[rev(order(df$y)),]
   x y
2 2 19
1 1 7
4 1 2
3 3 2
> quit()

What is shown above is a simple demo case on login nodes. For real interactive analysis scenario, users are encouraged to run on compute
nodes using the 'srun' command to request dedicated resources, e.g.:

$ srun --x11 --nodes=1 --ntasks-per-node=4 --mem=4000 -t2:00:00 --pty /bin/bash
$ xterm
$ module load r/intel/3.3.2
$ R

Besides running our analysis interactively, long running and big data crunching jobs ought to be submitted to the batch system slurm. The
"example.R" can be submitted to slurm to run in batch mode.

Copy example files to your newly created directory.
Below is how the example looks like:

```r
cp /share/apps/examples/r/basic/example.R /scratch/$USER/example
```

```r
$ cat example.R
df <- data.frame(x=c(1,2,3,1), y=c(7,19,2,2))
df
indices <- order(df$x)
order(df$x)
df[indices,]
df[rev(order(df$y)),]
```

Then create a sbatch job script as:

```bash
$ cat run-R.sbatch
#!/bin/bash

#SBATCH --job-name=RTest
#SBATCH --nodes=1
#SBATCH --tasks-per-node=1
#SBATCH --mem=2GB
#SBATCH --time=01:00:00
module purge
module load r/intel/3.3.2

cd /scratch/$USER/example
R --no-save -q -f example.R > example.out 2>&1
```

Once the sbatch script file is ready, it can be submitted to the job scheduler using sbatch. After successful completion of job, verify output log file for detail output information.

```bash
sbatch run-R.sbatch
```

(more...)

How do I run a Mathematica job?
(more...)

How do I start a multinode parallel job that is NOT MPI (eg Julia)?

The MPI modules on Mercer are built with support for the batch system. However, third-party MPI libraries and parallel software (such as Julia) may not be.

To launch a Julia job on multiple nodes you can use the node list provided by $PBS_NODEFILE:
For an MPI job that does not use the MPI modules on Mercer:

```
mpirun -np --machinefile $PBS_NODEFILE ./my_mpi_exec.exe
```

To run one multithreaded MPI process per node (hybrid MPI/OpenMP), see Running jobs - MPI.

Parallel libraries other than the MPI modules on Mercer do not normally have support for Torque, consequently they do not play nicely with other jobs. For this reason, the queue for multinode jobs sets the "#PBS -n" (node-exclusive) option. Multinode jobs therefore do not share nodes with any other job.

(thanks Spencer for the Julia tip!)

How can I view a PDF file on Prince?

```
evince myfile.pdf
```

You need to have logged in with X forwarding enabled, as evince is an X application. See Logging in to the NYU HPC Clusters for how to do this.

Managing Data

How much of my file/space quota have I used?

On Prince, enter ‘myquota’ at the prompt to see how much space you have used and available on each filesystem

How do I give my colleague access to my files?

An access control list (or ACL) gives per-file, per-directory and per-user control over who can read, write and execute files. You can see the ACL for a file or directory with the `getfacl` command:

```
$ getfacl myfile.txt
```

To modify permissions for files or directories, use `setfacl`. For a detailed description, see `man setfacl`. In the example below, I give read permission on dummy.txt to user bob123:

```
$ setfacl -m u:bob123:r myfile.txt
```

For setting execute permission on files `chmod` (more...)

How do I get the best transfer speed to or from BuTinah?

For faster transfer between the HPC clusters at NYU in NYC and the BuTinah cluster at NYUAD, use `scp` over port 922. This will route the transfer over a high bandwidth ANKABUT link rather than the default low bandwidth MLPS link. The speed difference is greatest when pulling files from BuTinah to NYU NY.

Transferring many small files will still be slow - you will get better performance if you tar small files into a single archive, and transfer the tar file.

The default user environment on bowery sets an alias for `scp` which does this automatically, so in most cases you can skip over this section. If you are finding that file transfers between NYUAD and NYU are slow, you can check whether you are using the alias with `which scp`. If the response is not "/usr/local/bin/scp_wrapper.sh", you should follow the instructions below.

You can `scp` over port 922 directly with the following commands, initiated from any of the NYU HPC clusters in NYC:

**Pushing to BuTinah:**
```

```

**Pulling from BuTinah:**
```

```
I have an huge amount of data that I want to compress for storage or transfer

Mercer has 'pigz', which is a parallel version of gzip. To use it:

```bash
module load pigz/intel/2.3.1
pigz --help
```

My workflow uses thousands of small files, how should I manage them

Managing large numbers of files

Filesystems generally - and high-performance filesystems such as Lustre especially - perform best with a small to moderate number of medium to large files. Some specific issues to be aware of are:

On $SCRATCH

- Lustre ($SCRATCH) gets performance mainly by striping distributing a large file across several disks and several "object storage servers". File metadata operations, on the other hand, do not have much parallelism available. So a few large read or write operations is vastly faster than many small reads or writes. This is true for reads and writes within a single files as well as for reads or writes on many files.
  - If your job does many small I/O operations, it might be better to copy the file to $PBS_JOBTMP or $PBS_MEMDISK at the start of the job, and open the local copy of the file.
  - (But for large reads and writes, $SCRATCH is likely to be faster than local disk)

- The default stripe count on $SCRATCH is 4, so each file is striped across disks on 4 object storage servers. If you have a folder filled with files each smaller than 1MB, it is better not to stripe them. You can set the stripe count on a folder (under $SCRATCH) to 1 with:

  ```bash
  lfs setstripe -c 1 $SCRATCH/folder_with_small_files/
  ``

- Finding a file within a folder is a serial operation. And the more files in a folder, the longer it takes. With several thousand files, even 'ls' on that folder can take several minutes and may affect responsiveness of the filesystem for other users.
  - If you have more than about 1000 files in one folder, distribute them over a number of subfolders. The best performance will be when the number of subfolders is the square root of the total number of files (eg, for 1 million files, 1000 subfolders each containing 1000 files)

On $ARCHIVE

- The backup regime on /archive is optimized for small numbers of large files - 1000 files of 1kb each take 1000 times as long to backup as 1 file of 1MB! Too many small files can prevent the backup from completing in time
  - when archiving a collection of small files, please `tar` the files first. You can send a collection of files to /archive with the command:

    ```bash
    # to archive $SCRATCH/my_run_dir
    tar cvf $ARCHIVE/simulation_01.tar -C $SCRATCH my_run_dir
    ```

    And fetch it again with:

    ```bash
    # to unpack it back into $SCRATCH/my_run_dir
    tar xvf $ARCHIVE/simulation_01.tar -C $SCRATCH
    ```

I want to keep a folder on the HPC cluster in sync with a folder on my workstation

- To replicate on Mercer a data directory you have on your workstation - assuming you are entering these commands **on a local**
**terminal on your workstation**, and you have an SSH **Tunnel** set up and running:

```bash
$ hostname
$ ls -F
$ rsync -av my_input_data mercer:/scratch/$USER/my_run_dir
```

The host name followed by a colon tells rsync that the (in this case) destination is on another host. If your username on the other host is different to the username on the current host, you can specify the remote username with `username@remotehost`:

**Note** the backslash in `\$USER` - this instructs the shell not to expand `$USER` to your local (on your workstation) username. An equivalent command is:

```bash
$ ls -F
$ rsync -av my_input_data NetID@mercer:/scratch/NetID/my_run_dir
```

- To copy in the other direction, from `/scratch` on Mercer to your workstation (again, from a local terminal on your workstation and across an SSH **Tunnel**):

  ```bash
  $ hostname
  $ ls -F
  $ rsync -av /scratch/$USER/my_run_dir my_results
  $ ls my_results
  ```

Only those files not already up-to-date on your workstation will be copied.

Click here for more about using rsync on the NYU HPC clusters

How do I transfer files to Dumbo cluster from Windows workstation?

First, download and install WinSCP tool from [here](#). If you are inside NYU network (on campus), simply open WinSCP and fill in all the fields:

![Login](image)

If you are outside of NYU network, one option is to **set up and use VPN**. After that you can use WinSCP as described above. Another option is to **start an SSH tunnel** on the workstation. We have instructions on how to do this for Windows workstations. Once your SSH tunnel is set up and started on dumbo, open WinSCP and fill the fields in as shown below:

![Login](image)