Using HPC

Obtaining an account
Unlike many other IT services, HPC access is by request only. If you have not yet obtained an account, or your account has expired, please submit an account request.

Prerequisites
You will need to be comfortable using a Unix/Linux command line after logging in with SSH.

Logging in
The subcluster pages will tell you which "front-end" server to log in to, depending on which hardware you want to use. Generally, you must log in to the HPC systems from the campus network (at W&M or VIMS), via the College’s VPN, or via a host that is on the campus network (such as stat.wm.edu, accessible from off-campus with your WMuserid and password) or you will see errors like Connection timed out or Network is unreachable. Chesapeake is behind VIMS (more restrictive) firewall and from W&M must be accessed via stat or by first logging into SciClone.

Running calculations
The login servers are called “front-ends” because you do not run your calculations there, but rather on back-end "compute" servers that the front-end server provides access to. Access compute servers via the batch system, using the qsub command.

In order to use installed software, you must generally "load" it using Environment Modules, or you will see errors like Command not found. We have specific guidance for users of MATLAB, Python, and other software under our Tutorials and Software pages, as well as for users compiling software themselves.

If you need to work with or produce more than a few gigabytes of data, familiarize yourself with filesystems other than your home directory, and with preventing your disk usage from disrupting others’ work.

When you are finished
The HPC systems cannot provide archival or long-term storage. If files no longer need to be available for work on the system, copy them off and delete them so that the space can be used for active projects. All files will be completely and permanently deleted after your HPC account expires, so if your files need to remain available for work on the system, keep track of when your account will expire, and before it expires either renew your account or contact us to arrange to have your files reassigned to another user.

Important topics:
• Getting an account
• Linux command line / text editors
• Logging into the clusters
• Selecting software
• How to use filesystems efficiently
• How to use the batch system
• Compiling / installing your own applications

HPC ticket system
mail: hpc-help@wm.edu

https://hpc.wm.edu OR
https://www.wm.edu/offices/it/services/hpc/atwm/index.php
Logging In

Must use Secure Shell client (SSH)
- Linux / Mac built-in (terminal)
- Windows – SSH Secure Shell Client / PuTTY

```
[ewalter@particle ~]$ ssh hurricane.sciclone.wm.edu
Password:
Last login: Tue Feb  2 13:57:59 2016 from particle.hpc.wm.edu
----------------------------------------------------------------------------
William and Mary Information Technology / SciClone Cluster
.
 i [hurricane]
```

Questions to ask yourself:

- Am I on or off campus?
  If you are off-campus
    - log into stat.wm.edu first using your W&M username and password

- Is my username the same as my current machine?
  If it is different use: ssh <username>@<host>.<domain>

- Do I need graphics?
  If yes, then log in with -X
Start-up Files & Modules

Start-up files control global and cluster specific settings

<table>
<thead>
<tr>
<th>File Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>.cshrc</td>
<td>personal environment settings for all subclusters</td>
</tr>
<tr>
<td>.cshrc.storm</td>
<td>for Hail, Ice, and Wind</td>
</tr>
<tr>
<td>.cshrc.rhel6-xeon</td>
<td>for Hurricane, Whirlwind, &amp;c.</td>
</tr>
<tr>
<td>.cshrc.rhel6-opteron</td>
<td>for Vortex and Potomac</td>
</tr>
<tr>
<td>.cshrc.rhel7-opteron</td>
<td>for Pamunkey</td>
</tr>
<tr>
<td>.cshrc.el7-xeon</td>
<td>for Bora, Hima, &amp;c.</td>
</tr>
<tr>
<td>.cshrc.el7-phi</td>
<td>for Meltemi</td>
</tr>
<tr>
<td>.cshrc.el7.x86_64</td>
<td>for James</td>
</tr>
</tbody>
</table>

Using start-up files is the recommended way to select software for particular cluster

$PLATFORM variable:

11 [vortex] echo $PLATFORM
rhel6-opteron

This means that startup is controlled by .cshrc.rhel6-opteron for vortex
**Modules and Start-up**

12 [vortex] module avail

------------------------------ /usr/local/Modules/modulefiles -------------------------------
acml/5.3.1/gcc                      mongo/2.6.12
acml/5.3.1/open64                   mpfr/3.1.3
acml/5.3.1/mpi                      mpi4py/2.0.0/gcc-5.2.0
acml-int64/5.3.1/gcc                mpi4py/3.0.0/gcc-5.2.0
acml-int64/5.3.1/open64             multiwell-2017/gcc
acml-int64/5.3.1/mpi                mvapich2-ib/2.2/gcc-5.2.0
acml-mp/5.3.1/gcc                   mvapich2-ib/2.2/intel
acml-mp/5.3.1/open64                mvapich2-ib/2.2/pgi-17.7
acml-mp/5.3.1/mpi                   mvapich2-tv-ib/2.2/gcc-5.2.0
acml-mp-int64/5.3.1/gcc             mvapich2-tv-ib/2.2/intel
acml-mp-int64/5.3.1/open64          mvapich2-tv-ib/2.2/pgi-17.7
.
.
.

13 [vortex] echo $PLATFORM
rhel6-opteron

14 [vortex] less .cshrc.rhel6-opteron

# # Environment configuration for RHEL 6.x / Opteron environment.
#
# #----------------------
# # VORTEX
# #----------------------
module load isa/seoul  
module load espresso/6.1/intel

16 [vortex] ml
Currently Loaded Modulefiles:
  1) modules  4) isa/seoul  7) espresso/6.1/intel
  2) maui/r156-GRes  5) intel/2017
  3) torque/6.1.1.1  6) openmpi/2.1.1/intel

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**isa controls which software stack is used**

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**Must start new session (log out and back in) to load new start-up modules**

http://www.wm.edu/offices/it/services/hpc/using/modules/index.php - online module help
Files and I/O

There are multiple file-systems available

Some are for ongoing / project storage **data, homeXX**

Some are for running jobs **scrXX, pscr**

**Only** data/homeXX backed up

Use local scratch when possible (every node has some)

Users are responsible for using disk space responsibly!!

Misuse of file-systems can disturb other jobs and can result in an administrative action!

Don't use data10 for job writes or large job reads

Use scratch space for jobs (90 day purge)

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**Summary of W&M HPC public user filesystems**

<table>
<thead>
<tr>
<th>Name</th>
<th>Appropriate for</th>
<th>Backups</th>
<th>Purged</th>
<th>Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>/sciclone/home10</td>
<td>Source code, executables, configuration files, scripts, and small (&lt;1GB total) data files. Unless you have been directed otherwise, <strong>you should not have a job read or write any substantial amount of data to your home directory</strong>, as doing so is extremely likely to impact others' interactive work.</td>
<td>Weeknightly, <strong>on-site only</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>/sciclone/home20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>/ches/home00</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>/sciclone/data10</td>
<td>Data that are needed on an ongoing basis for active projects on the cluster and cannot be easily re-created or re-uploaded. <strong>Please do not have batch jobs write a substantial amount to data filesystems. Please use the scratch filesystems for job output unless already given permission from HPC staff.</strong></td>
<td>Weekly, <strong>on-site only</strong></td>
<td>After account expiration,</td>
<td>Low</td>
</tr>
<tr>
<td>/ches/data10</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>/sciclone/scr10</td>
<td><strong>Scratch space:</strong> job outputs and working data that can be easily re-created or re-uploaded, or which will be copied elsewhere for longer-term storage.</td>
<td><strong>Never</strong></td>
<td>Any files not accessed for 90 days, and after account expiration.</td>
<td>Medium</td>
</tr>
<tr>
<td>/local/scr</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>/ches/scr10</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>/sciclone/scr10</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>/sciclone/scr20</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>/sciclone/pscr</td>
<td></td>
<td></td>
<td></td>
<td>High</td>
</tr>
</tbody>
</table>

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https://www.wm.edu/offices/it/services/hpc/using/files/index.php
Transferring Files

Each file-system has a server that runs it
For direct access you are STRONGLY encouraged to use the recommended node

e.g. : Logged into bora ; cd’d into data10 ; transfer off-site

Do this from tempest since files won't have to hop through bora to get off-site.

Globus - https://www.globus.org/
We have direct endpoints for most file-systems
Sharing Files & Folders: Permissions

see
https://www.nersc.gov/users/storage-and-file-systems/unix-file-permissions
for more information

33 [hurricane] pwd
/sciclone/home04/ewalter
print working directory

34 [hurricane] ls -ld results
Drwx------ 2 ewalter hpcf 512 Jun 16 14:37 results

**directories need to be ‘x’ to be entered/passed through

35 [hurricane] ls -l results
total 3
-rw------ 1 ewalter hpcf 194 Jun 16 14:37 ww.dat
-rw------ 1 ewalter hpcf 194 Jun 16 14:37 yy.dat
-rw------ 1 ewalter hpcf 194 Jun 16 14:37 zz.dat
list directory
list files in directory
**Common Permissions Tasks I**

### Change the permissions of a directory `chmod`:

```
[hurricane] ls -ld VASP
drwx------ 4 ewalter hpcf 512 Apr 4 2014 VASP
25 [hurricane] chmod go+rX VASP
26 [hurricane] ls -ld VASP
drwxr-xr-x 4 ewalter hpcf 512 Apr 4 2014 VASP
27 [hurricane] chmod o-rX VASP
28 [hurricane] ls -ld VASP
drwxr-x--- 4 ewalter hpcf 512 Apr 4 2014 VASP
29 [hurricane] chmod g-rX VASP
30 [hurricane] ls -ld VASP
drwx------ 4 ewalter hpcf 512 Apr 4 2014 VASP
```

### Change the permissions of a directory and everything under it `chmod -R`:

```
32 [hurricane] ls -ld VASP
drwx------ 4 ewalter hpcf 512 Apr 4 2014 VASP
33 [hurricane] ls -l VASP
total 52457
-rw------- 1 ewalter hpcf 22932904 Apr 4 2014 potpaw_LDA.52.tar.gz
-rw------- 1 ewalter hpcf 25958479 Apr 4 2014 potpaw_PBE.52.tar.gz
drwx------ 2 ewalter hpcf 15360 Aug 6 00:01 vasp.5.3
34 [hurricane] chmod -R g+rX VASP

35 [hurricane] ls -ld VASP
drwxr-x--- 4 ewalter hpcf 512 Apr 4 2014 VASP
36 [hurricane] ls -l VASP
total 52457
-rw-r----- 1 ewalter hpcf 22932904 Apr 4 2014 potpaw_LDA.52.tar.gz
-rw-r----- 1 ewalter hpcf 25958479 Apr 4 2014 potpaw_PBE.52.tar.gz
drwxr-x--- 2 ewalter hpcf 15360 Aug 6 00:01 vasp.5.3
```

Use this command if you want to allow group access to your home, scrXX, and dataXX directories.
Common Permissions Tasks II

How do I change the initial permissions that files and folders are given when created:

You need to edit your .cshrc file in your home directory and add: `umask`

- `umask 077` files get “-rw----------” folders get “drwx----------”
- `umask 027` files get “-rw-r------” folders get “drwxr-x-----”
- `umask 022` files get “-rw-r-r---” folders get “drwxr-xr-x”

HPC default umask is 077

What groups am I in?: `groups`

52 [hurricane] groups ewalter
ewalter : hpcf wmall hpcstaff www seadas vasp sysadmin wm hpcadmin wheel hpsmh

My primary (default) group is hpcf and the rest are secondary

Change a group associated with a file or directory: `chgrp`

54 [hurricane] ls -1d project
drwx------ 2 ewalter hpcf 512 Aug 18 20:47 project
55 [hurricane] chgrp hpcstaff project
56 [hurricane] ls -1d project
drwx------ 2 ewalter hpcstaff 512 Aug 18 20:47 project
Software and Compilers

There are many software packages available on the HPC systems! Ways to find out whether a package is available

- Check the modules on a particular cluster with: “module avail”
- Look at software web page (http://hpc.wm.edu/software/)
- Install it yourself
- Email hpc-help@wm.edu

We encourage users to install their own software in their home directory if possible. We will also do it for you or at least help, but we get LOTS of request so try not to abuse.

- Compilers: Intel, PGI, GNU
- MPI libraries: Intel, mvapich2, openmpi
- mvp2run – wrapper for all three with extra functionality (node load checking)

https://www.wm.edu/offices/it/services/hpc/using/jobs/mvp2run/index.php
Using the Batch System

HPC uses Torque (PBS) to schedule and run jobs. Nodes are selected via the `node type` `qsub` – submits the job to the batch system

```bash
27 [vortex] qsub -I -l walltime=30:00 -l nodes=1:vortex:ppn=12
```

```
qsub: waiting for job 1552781 to start
qsub: job 1552781 ready
```

```bash
1 [vx01] python prog.py
```

**Interactive** job puts you on a node ready to work

There are many *node types*. The default node type is simply the sub-cluster name *vortex*

It is also possible to select certain subsets within a cluster or a collection of sub-clusters

- `x5672` – any hurricane or whirlwind node
- `c18b` – only large memory vortex nodes

See online documentation or send email to `hpc-help@wm.edu` for more information

https://www.wm.edu/offices/it/services/hpc/hw/nodes/index.php
https://www.wm.edu/offices/it/services/hpc/using/jobs/index.php

**DO NOT RUN JOBS ON FRONT-END/LOGIN MACHINES!**
You can also submit a **batch** job which does not run interactively.

First you must write a **batch script**:

```
#!/bin/tcsh
#PBS -N test
#PBS -l nodes=1:x5672:ppn=8
#PBS -l walltime=0:10:00
#PBS -j oe

cd $PBS_O_WORKDIR
python prog.py >& prog.out
```

**Listing 1**

```
#!/bin/tcsh
-N
-l
-j

cd $PBS_O_WORKDIR
./a.out
```

**Listing 2**

- `#PBS -N test`: name of the job
- `#PBS -l nodes=1:x5672:ppn=8`: job specifications (nodespec)
- `#PBS -l walltime=0:10:00`: combine stderr and stdout
- `#PBS -j oe`: cd to where I submitted the job
- `python prog.py >& prog.out`: run the job

---

**Command Reference**

- `qsub`: submit job
- `qdel`: delete job
- `qstat`: list jobs
- `qsu`: list my jobs

---

**Warning**

```
Warning: no access to tty (Bad file descriptor).
Thus no job control in this shell.
tput: No value for $TERM and no -T specified
```
Using the Batch System III

MATLAB example

```bash
#!/bin/tcsh
#PBS -N test
#PBS -l nodes=1:x5672:ppn=8
#PBS -l walltime=12:00:00
#PBS -j oe
#PBS -q matlab

cd $PBS_O_WORKDIR
module load matlab

matlab -nodisplay -r "readMatrix" >& OUT
```

must add -q matlab for matlab jobs
load matlab module (if needed)
redirect stdout and stderr
file for stdout and stderr

```matlab
108 [hurricane] head readMatrix.m
tic
%parpool(8)
syms a b c d;
meshpoints = meshgenerator();
eigfile = fopen('eigfile.txt', 'wt');
count = 1;
count2 = 1;
%set(0, 'CurrentFigure', 1);
%plot3(0,0,0,'.');
%grid on . .
```

https://www.wm.edu/offices/it/services/hpc/using/jobs/submitting/index.php
Where to get help?

HPC webpage: [http://www.wm.edu/offices/it/services/hpc/atwm/index.php](http://www.wm.edu/offices/it/services/hpc/atwm/index.php)
HPC ticket system mail: [hpc-help@wm.edu](mailto:hpc-help@wm.edu)

Using the ticket system is useful since it is monitored by three of us

WE'RE HERE TO HELP!
Q&A