Introduction to the Cluster

Advanced Computing Center for Research and Education
http://www.accre.vanderbilt.edu
Our cluster is a little different than most...

* Most clusters are bought all at once.
* Therefore, all of the nodes are identical.
* Our cluster has evolved over time; it started with 120 dual-CPU P4's (and was ranked at #199 on the June 2003 "Top 500" list - http://www.top500.org).
* The cluster has grown over time as researcher demand has dictated.
* Older nodes have been "retired."
* It is now comprised of more than 700 nodes / 7000 processor cores, which isn't enough to even make the "Top 500" list now (The current #1 system has over 3 million cores).
## Compute Node Types

<table>
<thead>
<tr>
<th>Processor Type</th>
<th># of cores per node</th>
<th>RAM per node</th>
<th># of GPUs / cores per GPU</th>
<th># of nodes in cluster</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dual-quads AMD Opteron</td>
<td>8</td>
<td>64 GB</td>
<td>N/A</td>
<td>60</td>
</tr>
<tr>
<td>Dual-quads Intel Xeon Westmere</td>
<td>8</td>
<td>24 - 128 GB</td>
<td>N/A</td>
<td>299</td>
</tr>
<tr>
<td>Dual-hex Intel Xeon Westmere</td>
<td>12</td>
<td>48 - 64 GB</td>
<td>N/A</td>
<td>91</td>
</tr>
<tr>
<td>GPU nodes Intel Xeon Westmere</td>
<td>8</td>
<td>48 GB</td>
<td>4 / 480</td>
<td>48</td>
</tr>
<tr>
<td>Dual-hex Intel Xeon Sandy Bridge</td>
<td>12</td>
<td>128 - 256 GB</td>
<td>N/A</td>
<td>200</td>
</tr>
</tbody>
</table>
If you have your laptop with you, please feel free to try all of these things out as we go along...

To log on - ssh vunetid@vmplogin.accre.vanderbilt.edu

You will be randomly assigned to one of our more than 1 dozen gateways via DNS round-robining.

To change your password, after logging on to one of the gateways, rsh auth and once logged in there change your password by executing passwd.

Please do not use your e-password as your cluster password (or vice versa).

It is not permissible to share passwords to an account. Doing so may result in the account being suspended.
You are permitted to use ssh key pairs to log on to the cluster.
Most ssh clients support key pairs.
You should use the cluster to generate your public / secret key pair.
You must password protect your secret key!!!
If you do not password protect your secret key then anyone who hacks your client machine (it has happened!) will have access to all of your files stored on the cluster.
For more information on using ssh key pairs see: http://www.ibm.com/developerworks/library/l-keyc/index.html
Displaying graphics over the network can be very slow and should therefore only be done when necessary (ex: using the DDT debugger to debug an application).

Linux and Mac clients - `ssh -X vunetid@vmplogin.accre.vanderbilt.edu`

Mac users may be prompted to install X11 if not done previously.

Windows clients require X-Window emulation software (ex: Reflection X or Hummingbird Exceed).

```
Nikkis-laptop$ ssh -X nikki@vmplogin.accre.vanderbilt.edu nikki@vmplogin.accre.vanderbilt.edu's password:
ACCRE Cluster

IMPORTANT -- IMPORTANT -- IMPORTANT -- IMPORTANT -- IMPORTANT --
If you are logging in to change your password, you must do
rsh auth
to get to the correct server. Do NOT use vmpsched.
-- ACCRE Staff --
$ setpks -a ddt
$ ddt
```
Cluster Storage

- Home directories (/home), scratch space (/scratch), and (optional) additional data storage (/data) are shared across all nodes in the cluster via IBM’s General Parallel Filesystem (GPFS).

- [http://www.accre.vanderbilt.edu/?page_id=63#gpfs](http://www.accre.vanderbilt.edu/?page_id=63#gpfs)

- /home and /data are backed up nightly to tape; /scratch is not.

- If possible, use /tmp on the individual compute nodes for temporary storage while your job is running; ~30+ GB of space per core.

- When your job is done, move results back to /data, /home or /scratch and clean up /tmp.
Default Disk Quotas

* For the /home filesystem...
  * Default disk quotas are 10 GB, with a 20 GB hard limit and a 7 day grace period.
  * Default file quotas are 100,000 files, with a 200,000 file hard limit and a 7 day grace period.

* For the /scratch filesystem...
  * Default disk quotas are 25 GB, with a 100 GB hard limit and a 14 day grace period.
  * Default file quotas are 100,000 files, with a 1,000,000 file hard limit and a 14 day grace period.

* There are no default quotas for the /data filesystem since quota there is only available via purchase.
Disk Quotas

- GPFS will allow you to exceed your quota for the duration of your grace period; after that, your quota becomes your hard limit.
- GPFS will not allow you to exceed your hard limit; attempting to do so will result in an I/O error.
- You can check your quota usage at any time with the `mmlsquota` command (located in `/usr/lpp/mmfs/bin`).
- Example: `mmlsquota --block-size auto`
- `gpfs20 = /data, gpfs21 = /scratch, /gpfs22 = /home`.
- The `mmlsquota` command will not lie to you!
- Keep in mind that if you have copied data to a co-workers’ home directory you are still the owner of those files and they therefore still count against your quota.
-* Linux and Mac clients can use `scp`
-* Windows clients may require add on software such as the GUI `ssh` client from [http://www.ssh.com](http://www.ssh.com). Putty is another popular choice.
-* To copy a file from your client to the cluster: `scp my_file vunetid@vmplogin.accre.vanderbilt.edu:~/somedir`
-* To recursively copy files from the cluster back to your client: `scp -r vunetid@vmplogin.accre.vanderbilt.edu:~/mydata ./mydir`
-* `sftp` is also supported if you prefer it.
Shell Initialization Files

* `.bashrc` for the Bash shell
* `.cshrc` for the C shell
Two Very Important Environment Variables

* PATH is a colon delimited list of directories where the shell looks for commands.
* LD_LIBRARY_PATH is a colon delimited list of directories where the shell looks for libraries.
*setpkgs* was developed by ACCRE to make updating your PATH and LD_LIBRARY_PATH variables easy ... you just add the appropriate “package” to your environment and setpkgs takes care of the rest

*pkginfo* displays the packages which are available; there are lots of packages, so you may want to use *grep* to filter results

*Since setpkgs and pkginfo were developed by ACCRE, they will not be available on any other clusters you may use.*

*Example on next slide...*
This example shows using `pkginfo` to see which:

- compilers are installed
- versions of the GNU Scientific Library are installed
- versions of ATLAS are installed

```
$ pkginfo -l | grep compiler
pkginfo returns various compiler settings for the specified package or tool.
  versions to use for returning the various compiler settings.
gcc_compiler  GCC Compiler (4.6.1)
  intel_compiler  Intel 11 Compiler, including fortran
  llvm_compiler  LLVM/Clang (3.2)

$ pkginfo -l | grep gsl
  gsl_gcc  GNU Scientific Library (GCC) [gsl]
  gsl_intel GNU Scientific Library (Intel) [gsl]

$ pkginfo -l | grep atlas
  atlas  ATLAS Self-tuning BLAS (GCC) [blas]
  atlas_nehalem_gcc  ATLAS Self-tuning BLAS for Nehalem (GCC) [blas]
  atlas_nehalem_intel  ATLAS Self-tuning BLAS (GCC) [blas]
  atlas_x86-64_gcc  ATLAS Self-tuning BLAS (GCC) [blas]
  dakota_atlas_x86-64_gcc Dakota
  lapack_atlas  LAPACK with ATLAS (GCC) [lapack]
  lapack_atlas_nehalem_gcc  LAPACK with ATLAS for Nehalem (GCC) [lapack]
  lapack_atlas_nehalem_intel  LAPACK with ATLAS for Nehalem (Intel12) [lapack]
  lapack_atlas_x86-64_gcc  LAPACK with ATLAS (GCC) [lapack]
```
Adding packages

* `setpkgs -a package_name` adds a package to your environment.
Erasing a package

* `setpkgs -e package_name` erases a package from your environment.
* Notice that the GCC compiler is still part of the environment.
Re replacing Packages

*setpkgs -r package_name* erases all previously added packages from your environment and replaces them with the specified package.
Adding packages to your shell initialization file

*Packages added via `setpkgs` on the command line are just like aliases and variables defined on the command line - they are in effect only until you log out. Therefore, just like with aliases and variables, to make them permanent you add them to your `.bashrc` or `.cshrc`.

If you submit a job to the cluster without adding the package(s) it needs to your `.bashrc` or `.cshrc`, the job will fail!