INTRODUCTION TO THE CLUSTER
A **computer cluster** consists of a group of interconnected servers (**nodes**) that work together to form a single logical system.
<table>
<thead>
<tr>
<th>Single user</th>
<th>Many users</th>
</tr>
</thead>
<tbody>
<tr>
<td>On-demand resources</td>
<td>Resources upon availability</td>
</tr>
<tr>
<td>Few simultaneous processes</td>
<td>Many simultaneous jobs</td>
</tr>
<tr>
<td>Limited memory</td>
<td>Large memory</td>
</tr>
<tr>
<td>Small data storage capability</td>
<td>Big data storage capability</td>
</tr>
</tbody>
</table>

**WHY YOU SHOULD USE A CLUSTER**
The **cluster gateways** are the main entry point to the cluster. Multiple gateways in round-robin rotation to guarantee access.

- Manage and/or edit files
- Code development
- Jobs submission
- Lightweight debugging

**Custom gateways** are gateways paid by and dedicated to specific research groups. They differ from cluster gateways for:

- Restricted group access
- Users can run resources intensive processes

- Run resources intensive processes
Users can log into the cluster with a Secure Shell (ssh) client.

From a terminal:  

```
ssh vunetid@login.accre.vanderbilt.edu
```

### Full Ubuntu-based Bash shell

To install:

```
https://goo.gl/tAsj8U
```

⚠️ Windows 10 only
ACCOUNT CREDENTIALS

I forgot my password
or
My password is expired

How can I change my password?

Log into the cluster

From the terminal: `ssh auth`

From `auth`: `passwd`

When prompted, enter your new password

Type `exit` to disconnect from `auth`

Within 20 minutes your new password will be active

Open a helpdesk ticket:

www.accre.vanderbilt.edu/help

Do not use your VU E-password!
## The Compute Nodes

### Regular Nodes

*Dual multicore CPUs*

<table>
<thead>
<tr>
<th>Family</th>
<th>No. of cores</th>
<th>RAM / GB</th>
<th>No. of nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Haswell</td>
<td>12</td>
<td>128</td>
<td>41</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>128</td>
<td>73</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>256</td>
<td>38</td>
</tr>
<tr>
<td>Sandy Bridge</td>
<td>12</td>
<td>64</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>128</td>
<td>190</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>256</td>
<td>7</td>
</tr>
<tr>
<td>Westmere</td>
<td>8</td>
<td>24</td>
<td>56</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>128</td>
<td>21</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>48</td>
<td>35</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>64</td>
<td>24</td>
</tr>
<tr>
<td>Nehalem</td>
<td>8</td>
<td>24</td>
<td>24</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>48</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>96</td>
<td>13</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>6,632</strong></td>
<td><strong>61,536</strong></td>
<td><strong>554</strong></td>
</tr>
<tr>
<td>The Compute Nodes</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------------------</td>
<td>---</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Regular nodes</strong></td>
<td><strong>Accelerated nodes</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>Dual multicore CPUs</em></td>
<td>![Image of Xeon processors]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>![Image of Xeon processors]</td>
<td>![Image of Xeon Phi (KNC)]</td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>Random Access Memory</em></td>
<td>![Image of Nvidia GPUs]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>![Image of RAM]</td>
<td>![Image of Nvidia GPUs]</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>4 x Nvidia GPU</strong></td>
<td><strong>2 x Xeon Phi (KNC)</strong></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The scheduler

1. Execute user’s workloads in the right priority order
2. Provide requested resources on compute nodes
3. Optimize cluster utilization

Users do not access compute nodes directly!
GPFS and DORS are distributed parallel filesystems that allow users to get access to the same set of directories on all nodes and all gateways on the cluster.

<table>
<thead>
<tr>
<th></th>
<th>Nightly backup</th>
<th>Included with account</th>
<th>For purchase</th>
</tr>
</thead>
<tbody>
<tr>
<td>GPFS</td>
<td>✓</td>
<td>✓</td>
<td>✗</td>
</tr>
<tr>
<td>/home</td>
<td>✓</td>
<td>✓</td>
<td>✗</td>
</tr>
<tr>
<td>/scratch</td>
<td>✗</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>/data</td>
<td>✓</td>
<td>✗</td>
<td>✓</td>
</tr>
<tr>
<td>DORS</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>/dors</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Managed by Center for Structural Biology, supported by ACCRE.

Provides easy access to data from both desktops and cluster.
**GPFS STORAGE QUOTA**

**QUOTA:** When exceeded the user receives a warning message. Usage has to return below the quota within the **GRACE PERIOD**.

**LIMIT:** Cannot be exceeded. Automatically set to the actual quota usage when grace period expires.

<table>
<thead>
<tr>
<th>Data size</th>
<th>Number of files</th>
<th>GRACE PERIOD</th>
</tr>
</thead>
<tbody>
<tr>
<td>QUOTA</td>
<td>LIMIT</td>
<td>QUOTA</td>
</tr>
<tr>
<td>/home</td>
<td>15 GB</td>
<td>20 GB</td>
</tr>
<tr>
<td>/scratch</td>
<td>50 GB</td>
<td>200 GB</td>
</tr>
<tr>
<td>/data</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Can be purchased at 1 TB increments.
GPFS STORAGE QUOTA

**QUOTA:** When exceeded the user receives a warning message. Usage has to return below the quota within the **GRACE PERIOD**.

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---

Quota usage on GPFS is accounted in different ways.

- **/home** → **USER:** User ownership
- **/scratch** → **USER/GROUP:** User or group ownership
- **/data** → **FILESET:** Group’s data directory content
How can I check my current quota usage?

accre_storage

- Shows the current usage for all quotas associated with the user.

<table>
<thead>
<tr>
<th></th>
<th>usage</th>
<th>Space Quota</th>
<th>Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Home (user):</td>
<td>12.41G</td>
<td>15G</td>
<td>20G</td>
</tr>
<tr>
<td>Scratch (user):</td>
<td>36.23G</td>
<td>50G</td>
<td>200G</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>usage</th>
<th>Space Quota</th>
<th>Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>120304</td>
<td>200000</td>
<td>300000</td>
</tr>
<tr>
<td></td>
<td>180276</td>
<td>200000</td>
<td>100000</td>
</tr>
</tbody>
</table>
### How can I check my current quota usage?

`accre_storage`

- Shows the current usage for all quotas associated with the user.

<table>
<thead>
<tr>
<th></th>
<th>Usage</th>
<th>Space Quota</th>
<th>Limit</th>
<th>Usage</th>
<th>Files Quota</th>
<th>Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Home (user):</strong></td>
<td>20.01G</td>
<td>15G</td>
<td>20G</td>
<td>120304</td>
<td>200000</td>
<td>300000</td>
</tr>
<tr>
<td><strong>Scratch (user):</strong></td>
<td>93.45G</td>
<td>50G</td>
<td>200G</td>
<td>180276</td>
<td>200000</td>
<td>1000000</td>
</tr>
<tr>
<td><strong>Scratch (group):</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>accre</td>
<td>7.85T</td>
<td>9T</td>
<td>10T</td>
<td>287562</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td><strong>Data (fileset):</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>accre</td>
<td>6.11G</td>
<td>2T</td>
<td>3T</td>
<td>4538712</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
**DATA TRANSFER**

**scp source destination**

- Copy data from *source* to *destination*.
- Remote source or destination must be preceded by “vunetid@login.accre.vanderbilt.edu:”

```
scp local_path vunetid@login.accre.vanderbilt.edu:remote_path
```

```
scp vunetid@login.accre.vanderbilt.edu:remote_path local_path
```
DATA TRANSFER

WinSCP

https://winscp.net
Researchers should focus on the **science** behind the software they use.

**LMOD**

Lua-based framework that provides a convenient way to customize user’s environment through software modules.

- Supports all shells available on the cluster.
Software is organized in a tree structure and displayed accordingly to the loaded dependencies.
**Lmod - The Essentials**

- **module avail <mod>**
  - If no module is passed, print a list of all modules that are available to be loaded.
  - If a module is specified, show all available modules with that name.

- **module load mod1 mod2 ...**
  - Load the specified modules.

- **module unload mod1 mod2 ...**
  - Unload the specified modules.

- **module list**
  - Show all modules loaded in the current environment.

- **module purge**
  - Remove all loaded modules from the environment.
Lmod - A few shortcuts

---

module list $\rightarrow$ ml

module load mod1 $\rightarrow$ ml mod1

module unload mod1 $\rightarrow$ ml -mod1

module avail $\rightarrow$ ml av

---

“Traditional science is all about finding shortcuts”

Rudy Rucker
1. Only one version of a given software can be loaded at any time. 
   \textit{LMOD} will automatically unload previously loaded modules on name clash.

2. Incompatible programs are prevented to be loaded at the same time. 
   E.g. Anaconda2 / Anaconda3 / Python X.Y.Z

3. If the version is not specified, the default module is loaded for that software. 
   The default module corresponds to the most recent version available.

4. When unloading a module, Lmod does not automatically unload its dependencies. 
   In this way unloading a module will not break other loaded modules' dependencies.
Lmod - Searching for Modules

How can I search among the visible modules?

```
module avail pattern
```
- Show only the visible modules that contain the desired pattern.

How can I search through all the modules, even the non visible ones?

```
module spider pattern
```
- Search all the modules that contain the desired pattern.
Lmod - Save loaded modules

I always need the same set of modules. How can I have them loaded automatically?

**OPTION 1:**
Add module load statements in your ~/.bashrc file.

This is the primary cause of software errors for our cluster users!

**OPTION 2:**
Save loaded modules in named collections.

```
module save collection_name
```

• Save the list of current loaded modules in ~/.lmod.d/collection_name.

```
module restore collection_name
```

• Restore the desired named collection in the current environment.
All the dependencies are built from source with the available compilers.

The whole software stack will be (mostly) independent from OS libraries.

All non-essential dependencies are hidden for user clarity.

**module --show-hidden avail**

- Show all the visible modules, including hidden ones.

**module --show-hidden spider pattern**

- Search across all modules, including hidden ones.

To load a hidden module, the version must be specified.
SOFTWARE POLICIES

New compilers/MPI with relative software stacks are available every 12 months.

Software stacks older than 3 years will be removed.

What if the software I need is not available via Lmod?

ACCRE uses **EasyBuild** to build the software stack.

Open a ticket to request the installation.

If not available via EasyBuild, we will discuss the alternatives.
NEED MORE HELP?

1. Check our Frequently Asked Question webpage:
   www.accre.vanderbilt.edu/faq

2. Submit a ticket from the helpdesk:
   www.accre.vanderbilt.edu/help

3. Open a ticket to request an appointment with an ACCRE specialist.

DO NOT submit tickets in “Rush cluster”!
Rush tickets are for cluster-wide issues only.
It’s cluster tour time!
CONNECT WITH REMOTE DISPLAY SUPPORT

From a terminal:

```
ssh -X vunetid@login.accre.vanderbilt.edu
```

Install **XQuartz** and connect as for Linux.

www.xquartz.org

---

1. Install and launch **Xming**

www.sourceforge.net/projects/xming

2. Configure PuTTY