INTRODUCTION TO THE CLUSTER
A **cluster** is a bunch of computers that are networked together to perform intensive computing jobs.

*If it takes a long time to run on a laptop…*

*…it can run on ACCRE faster and with more memory, doing more in less time*
The cluster is downstairs!

You don’t need to be there to operate it, in fact we restrict physical access to the cluster and we only go there for maintenance.
## 10 Reasons to Use the ACCRE Cluster

<table>
<thead>
<tr>
<th>Reason</th>
<th>Benefit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Accessing larger processor or memory</td>
<td>It’s available anywhere</td>
</tr>
<tr>
<td>resources</td>
<td></td>
</tr>
<tr>
<td>Getting more done in less time</td>
<td>You can share files and results with others</td>
</tr>
<tr>
<td>It’s reliable</td>
<td>It’s reasonably priced</td>
</tr>
<tr>
<td>All the software is installed</td>
<td>It’s backed up</td>
</tr>
<tr>
<td>We’re here to help</td>
<td>We can handle sensitive data</td>
</tr>
</tbody>
</table>
In most cases you use a **SSH** client (**secure shell** client)
Starting ACCRE for the first time

Users can log into the cluster with a Secure Shell (ssh) client.

From a terminal:  

```
ssh vunetid@login.acre.vanderbilt.edu
```
You will need to set up a password if you haven’t already.

Password criteria is very strict!

- At least 14 characters long (but less than 4096)
- Perfect score on the ZXCVBN test
- You may use non-ASCII characters (emoji, Chinese, Japanese, Korean, etc.)
- This may cause issues with some terminal clients
- All characters must be printable and in UTF-8

If you need a password, type “accre_password generate”
ACCOUNT CREDENTIALS

How can I change my password?

1. Log into the cluster
2. Get a suggestion: `accre_password generate`
3. Change your password: `accre_password change`
4. When prompted, follow instructions
5. Your new password will be immediately active

I forgot my password
or
My password is expired

Open a helpdesk ticket:
www.vanderbilt.edu/accre/help

Do not use your VU E-password!
ACCOUNT CREDENTIALS

Use common sense!

- Choose a strong password
- Use a unique password for ACCRE, and do not use it for anything else
- If you write down your password, keep the note hidden and secure
- Consider using a password manager
- Never share your password with anyone for any reason
- If anyone asks for your password, report the incident to ACCRE and to VUIT security
- If you suspect your password is compromised, alert ACCRE and change it
The Visualization Portal allows for cluster access using any modern web browser:

- File management, upload, download, editing
- Shell access to gateways in browser
- View running jobs
- Spawn interactive desktop jobs on compute nodes
- Spawn Jupyter notebooks on compute nodes

WATCH VIDEO
STARTING THE VISUALIZATION PORTAL

Log into the Visualization Portal using an up to date web browser:
https://portal.accre.vanderbilt.edu

Check for browser updates and a valid site certificate before entering credentials!
DATA TRANSFER - PORTAL

Opens in a new browser tab
SHELL ACCESS TO THE CLUSTER - PORTAL

Opens in a new browser tab
REMOTE INTERACTIVE DESKTOP

- User enters resource requirements
- Desktop job submitted to scheduler
- User alerted when desktop is ready
Remote Interactive Desktop

Desktop opens in a new browser tab.

The desktop will persist between browser sessions.
DATA TRANSFER

Best way – use the file explorer on the ACCRE Visualization Portal!

If you must use a terminal:

```
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
Connect with Remote Display Support

Best way – create a virtual desktop on the ACCRE Visualization Portal to access graphical programs.

Remote displays on the terminal are slow and use up resources for other users.

If you must use a terminal:

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
Lmod

Lua-based module system

Allows you to run software packages and build environments based on them

Developed at Texas Advanced Computing Center
Software is organized in a tree structure and displayed accordingly to the loaded dependencies.
DIFFERENT WAYS TO LOAD PYTHON

Module load python
Module load Anaconda3
Module load GCC python
Module load Intel python

While helpful for beginners, Anaconda Python isn’t optimized for our hardware and can quickly use up the filesystem quota.

You will need to load the GCC or Intel module prior to loading the Python module. For starting out, GCC and Intel are interchangeable.
**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.
“Traditional science is all about finding shortcuts”

Rudy Rucker
<table>
<thead>
<tr>
<th>Number</th>
<th>Rule Description</th>
<th>Examples</th>
</tr>
</thead>
</table>
| 1      | Only one version of a given software can be loaded at any time. | module load GCC Python=3.7  
module load GCC Python=3.8 # unloads Python 3.7 |
| 2      | Incompatible programs are prevented to be loaded at the same time. | module load Anaconda3  
module load GCC Python # doesn’t work |
| 3      | If the version is not specified, the most recent version is assumed. | module load GCC Python # loads the latest GCC-compiled version of Python |
| 4      | When unloading a module, Lmod does not automatically unload its dependencies. | module load GCC Python  
module unload Python # GCC is still loaded |
**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.

**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.

This is the primary cause of software errors for our cluster users!
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.
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.
SLURM: Interface to the Compute Nodes

**User**
- https
- ssh

**Portal**

**Gateways**

**Scheduler**

**Compute Nodes**

**LDAP**

**Custom Gateways**

**L-Store**

**GPFS**

**DORS**
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 resource intensive processes
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 (unless requested via the portal)!
## The Compute Nodes

**Regular nodes**

**Dual multicore CPUs**

**Random Access Memory**

<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><strong>Skylake</strong></td>
<td>16</td>
<td>256</td>
<td>41</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td>128</td>
<td>52</td>
</tr>
<tr>
<td><strong>Haswell</strong></td>
<td>12</td>
<td>128</td>
<td>41</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>128</td>
<td>120</td>
</tr>
<tr>
<td></td>
<td>256</td>
<td></td>
<td>50</td>
</tr>
<tr>
<td><strong>Sandy Bridge</strong></td>
<td>12</td>
<td>64</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>96</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>128</td>
<td></td>
<td>193</td>
</tr>
<tr>
<td></td>
<td>256</td>
<td></td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>128</td>
<td>3</td>
</tr>
<tr>
<td><strong>Westmere</strong></td>
<td>8</td>
<td>128</td>
<td>22</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>48</td>
<td>16</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>8,292</td>
<td>82,432</td>
<td>575</td>
</tr>
</tbody>
</table>
# The Compute Nodes

<table>
<thead>
<tr>
<th></th>
<th>Family</th>
<th>No. of cores</th>
<th>RAM / GB</th>
<th>No. of nodes (GPUs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Newer</td>
<td>Nvidia Pascal</td>
<td>8</td>
<td>256</td>
<td>24 (96)</td>
</tr>
<tr>
<td></td>
<td>Intel Broadwell</td>
<td>8</td>
<td>256</td>
<td>24 (96)</td>
</tr>
<tr>
<td></td>
<td>Nvidia Maxwell</td>
<td>12</td>
<td>128</td>
<td>10 (40)</td>
</tr>
<tr>
<td></td>
<td>Intel Haswell</td>
<td>12</td>
<td>128</td>
<td>10 (40)</td>
</tr>
<tr>
<td></td>
<td><strong>Total</strong></td>
<td><strong>312</strong></td>
<td><strong>7,424</strong></td>
<td><strong>34 (136)</strong></td>
</tr>
</tbody>
</table>

- **Accelerated nodes**
  - Dual multicore CPUs
  - Random Access Memory
  - 4 x Nvidia GPU
  - 40 Gbit/s RoCE Network

**Older**

**Newer**
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>/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>
</tbody>
</table>

GPFS

Managed by **Center for Structural Biology**, supported by ACCRE.

Provides easy access to data from both desktops and cluster.
Rabo exceeded his quota on /scratch:

/scratch quota: **50 GB**
/scratch limit: **200 GB**
/scratch grace period: **14 days**

He has **14 days** to get /scratch below **50 GB**, and he can’t go above **200 GB**, or he won’t be able to add more data.
**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>15 GB</td>
<td>20 GB</td>
<td>200,000</td>
</tr>
<tr>
<td>50 GB</td>
<td>200 GB</td>
<td>200,000</td>
</tr>
</tbody>
</table>

Can be purchased at 1 TB increments.

Note that groups may also purchase additional scratch quota in 1 TB increments.
**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.

---

**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?

- Use the `accre_storage` command to show the current usage for all quotas associated with the user.

<table>
<thead>
<tr>
<th>Home (user):</th>
<th>Usage</th>
<th>Quota</th>
<th>Limit</th>
<th>Usage</th>
<th>Files</th>
<th>Quota</th>
<th>Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.41G</td>
<td>15G</td>
<td>20G</td>
<td></td>
<td>120304</td>
<td>200000</td>
<td>300000</td>
<td></td>
</tr>
<tr>
<td>Scratch (user):</td>
<td>36.23G</td>
<td>50G</td>
<td>200G</td>
<td>180276</td>
<td>200000</td>
<td>100000</td>
<td></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>Quota Type</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>Home (user)</td>
<td>20.01G</td>
<td>15G</td>
<td>20G</td>
<td>120304</td>
<td>200000</td>
<td>300000</td>
</tr>
<tr>
<td>Scratch (user)</td>
<td>93.45G</td>
<td>50G</td>
<td>200G</td>
<td>180276</td>
<td>200000</td>
<td>100000</td>
</tr>
<tr>
<td>Scratch (group): accre</td>
<td>7.85T</td>
<td>9T</td>
<td>10T</td>
<td>287562</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Data (filesystem): accre</td>
<td>6.11G</td>
<td>2T</td>
<td>3T</td>
<td>4538712</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
**FAIRSHARE/BURSTING LIMITS**

**showLimits -g group**

- Show the cluster resources limits for a specific *group*.

```
[vanzod@vmps09 ~]$ showLimits -g capra_lab
ACCOUNT         GROUP    FAIRSHARE MAXCPUS  MAXMEM(GB) MAXCPUTIME(HRS)
--------------- ------------ --------- --------- ----------- ---------------
capra_lab_account  16        272       2720       26112
               capra_lab    1        -          -          -
```

Users in the same group share the same amount of resources.
Provides live status on cluster usage and file system usage
NEED MORE HELP?

Overview

Cluster availability information

Cluster utilization, past 24h

Let us optimize your workflow
NEED MORE HELP?

Check the FAQs before submitting a ticket!

If you need software installed, use the Software Installation Request form

Rush tickets wake up the ACCRE on-call staff member. Only open a rush ticket if it affects all ACCRE users!
Basic Tutorial: One Million Digits of Pi

In this tutorial we will be using a Python script to calculate the first million digits of Pi using the ACCRE cluster. Although we will be using Python code, you don't need to know Python for this tutorial. However, you will need an ACCRE account and should be familiar with Linux commands.

If you haven't done so already, log in to ACCRE using a terminal.

Lmod

Complete the One Million Digits of Pi tutorial
vanderbilt.edu/accre/getting-started/tutorial

This isn’t required but it will give you a sense of how Lmod and SLURM work!
IT’S CLUSTER TOUR TIME!