FAQ

Frequently Asked Questions

Account Access

A step-by-step guide is available on our Account Creation page.

There are many reasons you may be having issues logging in. A list of possible reasons may include:

- You haven't created an account yet.
- Your account isn't sponsored yet.
- You aren't using two-factor authentication (NetID+).
- You need to wait 15 minutes. If you just created your account, it takes time before you can log in.
- You're trying to connect using ssh NetID@login.hpc.arizona.edu. This will not work. Instead, use: ssh NetID@hpc.arizona.edu.
- You're using NetID@hpc.arizona.edu or NetID@email.arizona.edu as your username in PuTTY. Instead, use only your NetID.
- You've entered your password incorrectly too many times. After multiple failed password entries, the system will place a 60 minute ban on your account for security reasons.

Linux systems do not display character strokes while entering your password which can make it look like the ssh client is frozen. Even though it doesn't appear that anything is happening, the system is still logging your input. To proceed, type your password at the prompt and press enter.

If you have just registered for an HPC account, you need to wait a little while for the request to propagate through the University systems (this can take up to an hour). Patience 😞

You need an HPC account - see our Account Creation page for details. Once you've done that, you'll need to wait a little while to log in. If your PI hasn't already added you to their group, you'll need to wait for that as well.

- Ensure you are using the correct password. Sometimes typing your password into a plain text file and copying/pasting it into the terminal can help.
- You need to wait about 15 minutes after your account is approved for the account to be available.
- You must enroll in NetID. Depending on the application you use to log in, you may not get the typical NetID+/DUO menu of options, or an error message indicating this is your problem.
HPC uses the same NetID login credentials as all UA services. If you need to reset your NetID password you can do so using the NetID portal: https://netid-portal.iam.arizona.edu/

Faculty members who manage their own HPC groups can follow the instructions in our Research and Class Groups page.

Yes, if you are a former university affiliate or campus collaborator participating in research, you may register as a Designated Campus Colleague (DCC). Once your DCC status has been approved, you will receive a NetID+ which you may use to create an HPC Account. If you already have an HPC Account, no further action is required.

General Computing

Perhaps your shell is not set to Bash. If you already had another account before joining HPC, that profile will carry over, while a brand new account will always default to bash. If your shell is not set to Bash, contact our consultants so that they can reset it for you.

When you log into HPC, the variable $COMMAND_PROMPT is set to your current cluster (e.g.: (puma)). Sometimes this can cause formatting problems. If you’d prefer to modify your $PS1, you can add the following to your ~/.bashrc:

```bash
if [ -n "$(PROMPT_COMMAND)" -a -r /usr/local/bin/slurm-selector.sh ]; then
  SavePS1=$(PROMPT_COMMAND)
  Cur_Cluster=$(eval $PROMPT_COMMAND 2>/dev/null)
  PS1="$(Cur_Cluster)$SavePS1"
  unset PROMPT_COMMAND
  for c in puma ocelote elgato; do
    alias $c="PS1=""\$(c) $SavePS1"
  done
  unset Cur_Cluster SavePS1
fi
```

These files are called core dumps and may be created when a program terminates abnormally. Core dumps contain the system’s memory at the time of the fault event as well as additional information that can be used with a debugger (e.g. gdb) to track down the source of the error.

One drawback to core dump files is they can be quite large. If you're working with limited space (e.g., your home directory or a nearly-full /groups or /xdisk) or are running many jobs, you may consider disabling them. To do this, include the following line in your batch script before your program's execution:

```bash
ulimit -c 0
```

Jobs and Scheduling

There are a few reasons your job may not be running, check below for some ideas on diagnosing the issue:

- Run `squeue --job <jobid>` and see if there is anything listed under "(REASON)". This may give an idea why your job is stuck in queue. We have a table in our SLURM documentation that describes what each Reason code means.

- Due to the number of HPC users, it may not always be possible to run a submitted job immediately. If there are insufficient resources available, your job will be queued and it may take up to a few hours for it to begin executing.

- Your group/job may have run out of standard hours. You can check your allocation using the command `va`.

- Your group/job has reached a resource usage limit (e.g., number of GPUs that may be used concurrently by a group, or a job has requested more than the 10 day max walltime). Try running `job-limits <group_name>` to see what limits you're subject to and if there are any problem jobs listed.

- You may be requesting a rare resource (e.g., 4 GPUs on a single node on Puma or a high memory node).
  - If you are requesting a single GPU on Puma and are frustrated with the wait times, you might consider checking if Ocelote will work for your analyses. There are more GPU nodes available on that cluster with shorter wait times.
  - If you are trying to run a job on a standard node and have been waiting for a very long time, try checking its status using `job-history <jobid>`. If you see Allocated RAM/CPU above 5gb on Puma or above 6gb on Ocelote, then you are queued for the high memory node which can have very long wait times. To queue for a standard node, cancel your job and check that your script has the correct ratios.
If your job is in queue, sometimes SLURM will give you information on why it's not running. This may be for a number of reasons, for example there may be an upcoming maintenance cycle, your group's allocation may be exhausted, you may have requested resources that surpass system limits, or the node type you've requested may be very busy running jobs. We have a list of reason codes in our Running Jobs With SLURM page that will give more comprehensive information on what these messages mean. If you don't see the reason code listed, contact our consultants.

If your jobs keep stopping and restarting, it's likely because you are using Windfall. Windfall is considered lower priority and is subject to preemption by higher priority jobs. Before submitting a job to Windfall, consider using your group's allotted monthly hours first. Jobs using Standard hours will queue for a shorter period of time and will not be interrupted. You can check your group's remaining hours using the command `va`. To see more information on your allotted hours and the different job queues, see: Allocation and Limits.

No. Software to run applications is not available on the login nodes. To run/test your code interactively, start an interactive session on one of the system's compute nodes. Processes running on the head node are subject to being terminated if we think they are affecting other users. Think of these as 'submit' nodes where you prepare and submit job scripts.

Unfortunately, that is not possible. The compute nodes get their image from the head node and have to remain the same. If you need to install software that needs root access, for example, you can install the software locally in your account. See this example.

SLURM will let you ssh to nodes that are assigned to your job, but not to others.

Specific Errors

This is most commonly seen with users who have Anaconda or Miniconda initialized in their accounts. For a permanent solution, you can run the following command from an interactive terminal session:

```
conda config --set auto_activate_base false
```

This will prevent conda from auto-activating when you first log in and allow you to have more control over your environment. When you'd like to activate anaconda, run `conda activate`. See this example for information running anaconda workflows in batch with auto-activation disabled.

Scripts created in a Windows environment and transferred to HPC retain hidden carriage returns (^M). You can convert your Windows file to Unix format with:

```
$ dos2unix <filename>
```

This happens most frequently for new users. It takes a while to propagate new accounts to all the right places. Come back after a coffee break. However, this can occur in other circumstances. Open a support ticket with hpc-consult.

Add this variable definition before executing the application:

```
export CUDA_FORCE_PTX_JIT=1
```

Software and Modules

Yes, when you start an interactive terminal session or submit a batch script, the modules ohpc, gnu8, openmpi3, and cmake are automatically loaded. If your code uses Intel compilers, you will want to manually unload gnu8 and openmpi3 to prevent conflicts.

The exception: If you are working in a terminal in an Open OnDemand interactive desktop session, nothing is loaded by default and you will need to manually load any necessary modules.

R installations can sometimes be frustrating. We have instructions for how to set up a usable R environment, how to diagnose and troubleshoot problems, and steps to help with known troublesome packages documented in our Using and Customizing R Packages section.

You may also want to take a look under our Popular Packages section in the page mentioned above. This includes instructions for packages that are known to cause issues for users.

You can install python packages locally using either a virtual environment or a local conda environment. See our documentation on using Python for instructions on how to set these up.
The current version of Singularity is 3.7.4. Prior versions have been removed, only the latest one is considered secure. Notify the consultants if you need help with transition to the current version. Singularity is installed on the operating systems of all compute nodes so does not need to be loaded with a module.

Load the module, find the path to the executable by checking the $PATH variable, then list the contents. For example:

```
module load lammps
echo $PATH
ls /opt/ohpc/pub/apps/lammps/3Mar20/bin
lmp_mpi
```

There are a few different possibilities:

- You are not in an interactive session. Modules are not available on the login nodes. You may request an interactive session by using the command `interactive`.
- Your shell is not set to bash. If this is the case, contact our consultants so that they can reset it for you.
- You have modified or deleted your ~/.bashrc. If this is the case, open (if the file exists) or create and open (if the file is missing) the file .bashrc in your home directory and add the lines:

  ```
  if [ -f /etc/bashrc ]; then
    . /etc/bashrc
  fi
  ```

If you are able to compile your software you can take advantage of most of the AMD Zen architecture.

<table>
<thead>
<tr>
<th>Compiler</th>
<th>Arch-Specific</th>
<th>Arch-Favorable</th>
</tr>
</thead>
<tbody>
<tr>
<td>GCC 9</td>
<td>-march=znver2</td>
<td>-mtune=znver2</td>
</tr>
<tr>
<td>LLVM 9</td>
<td>-march=znver2</td>
<td>-mtune=znver2</td>
</tr>
</tbody>
</table>

Neither of these compiler versions (GCC 9 or LLVM 9) is available on Puma so you will have to build that first. If you use GCC 8.3 you can set znver1 instead.

Unfortunately, Windows applications can't be run on HPC. However, AWS has been used successfully for Windows software with GPU needs. It's easy to set up, cost effective, and very scalable. Amazon also has a cloud credit for research program available [here](https://aws.amazon.com/government-education/research-and-technical-computing/cloud-credit-for-research/)

You may also consider trying Jetstream2, a national resource where you can create and use Windows virtual machines. More information can be found here: [here](https://jetstream-cloud.org/)

Intel compilers are optimized for Intel processors. There is some debate around the concept of unfair CPU dispatching in Intel compilers. By default, software on the HPC clusters is built with GCC (on Puma it is GCC 8.3). This is in keeping with our preference for community software.

You need to belong to a special group called g03. You can request to be added by submitting a help ticket. This is a constraint in Gaussian that other modules do not have.

Ansys has the Distributed capability built in to increase performance. Ansys uses the Intel compiler and so uses Intel MPI. By default, we load OpenMPI, so you will need to do this:

```
module unload gnu8 openmpi3
module load intel
module load ansys
```

Instructions on accessing custom packages are under [Accessing Custom Packages from a Jupyter Session](https://example.com) in our documentation on [Using and Installing Python & Python Packages](https://example.com).
Data Storage and Transfer

No. We NFS mount storage across all compute nodes so that data is available independent of which compute nodes are used. See this section for how to transfer data.

After creating your HPC Account, your home directory will not be created until you log in for the first time. Without your home directory, you will not be able to transfer your data to HPC. If you are struggling and receiving errors, sign into your account either using the CLI through the bastion or logging into OnDemand and then try again.

If you are using something like SCP and are receiving errors, make sure your hostname is set to filexfer.hpc.arizona.edu (not hpc.arizona.edu).

Unfortunately, no. Backups are not made and anything deleted is permanently erased. It is impossible for us to recover it. To ensure your data are safe, we recommend:

- Make frequent backups, ideally in three places and two formats. Helpful information on making backups can be found on our page Transferring Data.
- Use `rm` and `rm -r` with caution as these commands cannot be undone! Consider using `rm -i` when removing files/directories. The `-i` flag will prompt you to manually confirm file removals to make sure they can be deleted.
- You can open a support ticket to request assistance. Files that are deleted may not have been removed from the storage array immediately (though this is not guaranteed), don’t wait more than a few days.

Endpoint too busy: This is most commonly seen when users are transferring directories to Google Drive. This is because Google has user limits restricting the number of files that can be transferred per unit time. When many files are being transferred at once, that limit may be exceeded. Globus will automatically hold the transfer until the limit is reset at which point it will continue. One way to avoid this is to archive your work prior to the transfer (e.g. in .tar.gz form). Additionally, archiving will also speed up your transfers considerably, sometimes by orders of magnitude.

Fatal FTP Response, PATH_EXISTS: Globus is finicky about the destination endpoint. If you get this error, check to see whether duplicate files/directories exist at the destination. This can happen frequently with Google Drive as multiple files/directories can exist in the same location with the same name. If duplicates exist, try moving, removing, or renaming them and reinitiate the transfer.

In our last maintenance update on July 20th, one of the changes was to ensure HIPAA compliance on the Data Transfer Nodes (DTNs). This change included the insertion of required text:

Authorized uses only. All activity may be monitored and reported.

This change breaks SCP activity. Not in all cases but frequently with WinSCP, Filezilla and from a terminal. Terminal activity will likely still work from Linux or MacOS.

The solution is to not use SCP (SCP is considered outdated, inflexible, and not readily fixed) and to use a more modern protocol like SFTP and rsync. Info on using SFTP:

- Putty supports SFTP with the "PSFTP" command
- For FileZilla, in the Toolbar, click on Edit and Settings, then click on SFTP
- For Cyberduck, choose SFTP in the dropdown for protocols.

Choose SFTP (SSH File Transfer Protocol), and use filexfer.hpc.arizona.edu as the Server. May enter Username and Password, and unselect “Add to KeyChain”.

For Mac, Cyberduck can be used. For version 8.4.2, select Go then Disconnect before clicking on Quit Cyberduck.

The recent Cyberduck patch 8.4.4 has created problems with two-factor authentication which is required to access filexfer.hpc.arizona.edu. Adding a SSH Keys is suggested.

For Windows, WinSCP and FileZilla are recommended.
If your home directory is full and you can’t find what is taking up all the space, it’s possible the culprit is a hidden file or directory. Hidden objects are used for storing libraries, cached singularity/apptainer objects, saved R session, anaconda environments, configuration files, and more. It’s important to be careful with hidden, or “dot”, files since they often control your environment and modifying them can lead to unintended consequences.

To view the sizes of all the objects (including hidden) in your home, one quick command is `du -hs $(ls -A ~)`, for example:

```
[netid@junonia ~]$ du -hs $(ls -A ~)
32K    Archives
192M   bin
4.7G   Software
46M    .anaconda
1.9M   .ansys
4.0K   .apptainer
16K    .bash_history
4.0K   .bash_logout
4.0K   .bash_profile
12K    .bashrc
20M    ondemand
```

Clearing out unwanted objects, moving data to a location with more space (e.g. /groups or /xdisk), and setting different defaults for data storage (e.g., resetting your apptainer cache directory or setting new working directories for Python/R) can help manage your home’s space.

Unfortunately, without active university credentials it is not possible to access HPC compute or storage resources. External collaborators who need ongoing access may apply for Designated Campus Colleague, or DCC, status. This is a process done through HR and will give the applicant active university credentials allowing them to receive HPC sponsorship.

Otherwise, data will need to be moved off HPC and made available on a mutually-accessible platform. This may include (but is not limited to): Google Drive, AWS S3, Box, and CyVerse’s Data Store.

**xdisk**

A group’s PI owns the /xdisk allocation. By default, your PI has exclusive read/write/execute privileges for the root folder /xdisk/PI.

By default, members of a research group only have write access to their subdirectories under /xdisk/PI. If they so choose, a PI may allow their group members to write directly to /xdisk/PI by running one of the following commands:

<table>
<thead>
<tr>
<th>Command</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>$ chmod g+r    /xdisk/PI</td>
<td>Group members can see the contents of the directory with ls, but may not access it or make modifications (e.g. add, delete, or edit files/directories)</td>
</tr>
<tr>
<td>$ chmod g+rx   /xdisk/PI</td>
<td>Group members can access the directory and see files but cannot make modifications (e.g. add, delete, or edit files/directories)</td>
</tr>
<tr>
<td>$ chmod g+rwX  /xdisk/PI</td>
<td>Group members are granted full read/write/execute privileges.</td>
</tr>
</tbody>
</table>

When an /xdisk allocation is created, a subdirectory is automatically generated for and owned by each individual group member. If the directory /xdisk/PI does not have group privileges, group members may not access the root directory, but may access their individual spaces by:

```
$ cd /xdisk/PI/netid
```

If a user joins the group after the xdisk was created and /xdisk/PI is not writeable for group members, contact our consultants and they can create one.
Typically when an /xdisk allocation is created, it will automatically generate a directory for each group member. In the unlikely event that it doesn’t or, more commonly, a group member is added after the allocation has been created, either the PI may manually create a directory or, if the root directory is group writable, the user may create one themselves. If the group’s /xdisk does not have full group permissions, the PI may run:

```
$ mkdir /xdisk/PI/netid
```

then can reach out to our hpc consultants to request an ownership change.

No, the full /xdisk allocation is available for every member of the group. It’s up to group members to communicate with one another on how they want to utilize the space.

A group’s PI owns the /xdisk allocation. By default, your PI has exclusive read/write/execute privileges for the root folder /xdisk/PI.

/xdisk is a temporary storage space available to your research group. When it’s close to its expiration date, notifications will be sent to all members of your group. For detailed information on /xdisk allocations, see: Storage

/xdisks are managed by your group’s PI by default. This means if you want to request an /xdisk or modify an existing allocation (e.g., extending the time limit or increasing the storage quota), you will need to consult your PI. Your PI may either perform these actions directly or, if they want to delegate /xdisk management to a group member, they may do so by following the instructions under Delegating /xdisk Management Rights.

To modify your allocation's time limit or storage quota, your PI can either do so through the Web Portal under the Storage tab, or via the command line. If your PI would like to delegate management rights to a group member, they may follow the instructions under Delegating /xdisk Management Rights. Once a group member has received management rights, they may manage the allocation through our web portal.

If you're getting errors using /xdisk commands in a terminal session, check that you are on a login node. If you are on the bastion host (hostname: gatekeeper), are in an interactive session, or are on the filexfer node, you won’t be able to check or modify your /xdisk. When you are on a login node, your terminal prompt should show the hostname

```
$ hostname
```

If you’re trying to extend your group’s allocation but are seeing something like:

```
(puma) [netid@junonia ~]$ xdisk -c expire -d 1
invalid request_days: 1
```

for every value you enter, your /xdisk has likely reached its maximum time limit. To check, go to portal.hpc.arizona.edu, click Manage XDISK, and look at the box next to Duration. If you see 300, your allocation cannot be extended further.

If your allocation is at it's limit, you will need to back up your data to external storage (e.g., a local machine, lab server, or cloud service). Once your /xdisk has expired (either by expiring or through manual deletion), you can immediately create a new allocation and restore your data. Detailed /xdisk information can be found on our Storage page. You may also want to look at our page on Transferring Data.

No, once an /xdisk has reached its time limit it will expire. It’s a good idea to start preparing for this early by making frequent backups and paying attention to /xdisk expiration emails.

Once an /xdisk expires, all the associated data are deleted. Deleted data are non-retrievable since HPC is not backed up. It's advised to keep frequent backups of your data on different platforms, for example a local hard drive or a cloud-based service like Google Drive, or (even better) both!

**Onsite Rental Storage**

Rental storage can be requested by PIs through the user portal. A guide with screenshots can be found in our rental storage documentation.
No, rental storage is not mounted on the HPC login or compute nodes which means jobs cannot access /rental directly. Data stored in /rental need to be moved to /home, /groups, or /xdisk to be available.

AWS Tier 2 Storage

A PI must submit their group's storage request. The exception to this is if a group member has been designated xdisk/storage delegate. Delegates may submit a request on behalf of their PI by switching users in the user portal.

In most cases it will be in one business day.

Yes. Using Globus you can move data from Google Drive to S3.

You should check the Amazon site: https://aws.amazon.com/s3/pricing/?nc=sn&loc=4
As of March 2022:

- Frequent Access Tier, First 50 TB / Month $0.023 per GB
- Frequent Access Tier, Next 450 TB / Month $0.022 per GB
- Frequent Access Tier, Over 500 TB / Month $0.021 per GB

Not in the first release, but potentially as a future offering

Yes. The capacity used is recorded daily and the billing is a monthly average.

It is used for accounting purposes and used by your Department's finance specialist.

Yes, you can use the CLI (command line interface) for information about your usage

No, but you can track the usage and remove any data that should not be there.

Glacier is effectively large, slow disks and Deep Glacier is tape storage.

Amazon S3 will likely support what you do. Perhaps our consultants can help to rework your workflows.

You will not be charged for data ingress, egress or other operations.

Yes

Yes, for any question we use ServiceNow and can be reached with a support ticket.

The max file size is 5TB based on: https://docs.aws.amazon.com/AmazonS3/latest/userguide/qfacts.html

This alert is sent to notify you whenever your storage usage grows by 10% relative to the previous week. This ensures that you're aware of any unintended spikes and the potential resulting costs.

Secure Services

You will first need to request access. Follow the instructions in our Secure HPC page to see all the steps that are required.

It's possible you're not connected to the VPN. You will need to be connected to access any Soteria resources.

Official AWS FAQs are here: https://aws.amazon.com/s3/faqs/
The easiest way to transfer your data to Soteria is using Globus. We have a high assurance endpoint set up accessible under the endpoint UA HPC HIPAA Filesystems.

It depends.

You do not need your personal computer's Globus endpoint set to high assurance for the purposes of transferring data to Soteria using our UA HPC HIPAA Filesystems endpoint. HIPAA requires data transfer auditing. We log transfers on our DTN that use the HIPAA endpoint, regardless of the client's managed status.

If you are working with another institution/endpoint that only allows connections from high assurance endpoints, then you must enable High Assurance during your Globus Personal Connect configuration process. This requires that you are added to our Globus subscription which can be done by opening a support ticket to request help from our consultants. Your endpoint must be set to public to allow us to add you. Once you have been added, you may set your endpoint to private.