



Introduction to NSF NCAR HPC Resources

2026 CESM Tutorial

Rory Kelly
HPC Consultant

July 6, 2026

Getting Help

HPC Documentation - <https://ncar-hpc-docs.readthedocs.io>

**NCAR**
OPERATED BY UCAR

NCAR HPC Documentation

 Search

 GitHub
v26.03 ☆ 14 26

NCAR HPC Documentation

Getting Started

End User Agreement

Accounts >

Allocations >

VPN access

System Usage Policies

Data Retention Policies

Best Practices for Supercomputer Users

Acknowledging NCAR and CISL

Getting Help

Compute Systems and Services

Derecho >

Casper >

CIRRUS >

Open OnDemand >

JupyterHub >

NCAR | COMPUTATIONAL & INFORMATION SYSTEMS LAB

User Documentation for NSF NCAR High Performance Computing

This is the home of the user documentation for the NSF NCAR high-performance computing (HPC) and storage resources managed by CISL. It includes searchable information specific to HPC resources, storage systems, authentication procedures and others, as well as additional how-to articles and troubleshooting articles.

Selected Links

- [Getting Started](#)
- [Using Derecho](#)
- [Using Casper](#)
- [Using JupyterHub](#)
- [Getting Help](#)

Don't find what you need? Log in here to submit a help request: [NCAR Research Computing](#).

You need a CIT password to submit a request. Call **303-497-2400** if you don't have one.



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Consultant on Duty

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NSF NCAR HPC Documentation

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Consultant on Duty

Submit a ticket

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Getting Help

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The screenshot shows the NCAR HPC Documentation website. The header includes the NSF and NCAR logos, the title 'NCAR HPC Documentation', a search bar, and a GitHub link. The left sidebar lists navigation categories: 'Getting Started' (with sub-items like End User Agreement, Accounts, Allocations, VPN access, System Usage Policies, Data Retention Policies, Best Practices for Supercomputer Users, and Acknowledging NCAR and CISL), 'Getting Help', and 'Compute Systems and Services' (with sub-items like Derecho, Casper, CIRRUS, Open OnDemand, and JupyterHub). The main content area features the NCAR Computational & Information Systems Lab logo, the title 'User Documentation for NSF NCAR High Performance Computing', and a paragraph stating that this is the home for user documentation for NSF NCAR HPC and storage resources. Below this is a 'Selected Links' section with a list: 'Getting Started', 'Using Derecho', 'Using Casper', 'Using JupyterHub', and 'Getting Help'. Three red arrows point from text labels to specific links: 'Consultant on Duty' points to 'Getting Help', 'Submit a ticket' points to 'NCAR Research Computing' in the text 'Log in here to submit a help request: NCAR Research Computing.', and 'Password Help' points to 'You need a CIT password to submit a request. Call 303-497-2400 if you don't have one.'

NSF NCAR HPC Documentation

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Compute Systems and Services

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Topics to Cover

- Available systems and their uses
- Signing in and managing data
- Accessing software
- Managing jobs using Batch schedulers
- Customizing your user environment

This is only an introduction; for full documentation, see:

<https://ncar-hpc-docs.readthedocs.io/en/latest/>

Derecho - Primary HPC Resource

- HPE Cray EX, 19.87 petaflops
- 2488 CPU Nodes
 - Dual socket, 64-core AMD 7763 “Milan” CPUs
 - 256 GB DDR4 Memory
 - 1 Cassini Slingshot-11 NIC
- 82 GPU Nodes
 - Single socket, 64-core AMD 7763 “Milan” CPUs
 - 512 GB DDR4 Memory
 - 4 NVIDIA A100 GPUs
 - NVLink GPU interconnect
 - 4 Cassini Slingshot-11 NICs



Casper - Data Analysis, HTC, Visualization

- 22 nodes for data analysis and visualization jobs. Each node has 36 cores and up to 384 GB memory.
 - 9 of these nodes also feature an NVIDIA Quadro GP 100 GPU.
- 18 nodes feature large-memory, dense GPU configurations to support explorations in machine learning (ML) and GPU computing
 - 4 of these nodes feature 4 NVIDIA Tesla V100 GPUs
 - 6 of these nodes feature 8 NVIDIA Tesla V100 GPUs
 - 8 of these nodes feature 4 NVIDIA Ampere A100 GPUs
- 64 high-throughput computing (HTC) nodes for small computing tasks using 1 or 2 CPUs.
 - 62 HTC nodes have 384 GB of available memory
 - 2 HTC nodes have 1.5 TB of available memory
- 4 nodes are reserved for Research Data Archive workflows

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TOO COMPLICATED FOR A SLIDE!

**If you really
want to know...**

<https://ncar-hpc-docs.readthedocs.io/en/latest/compute-systems/casper/#casper-hardware>

System Access - Duo Authentication

You should have received an email to set up **Duo** Authentication

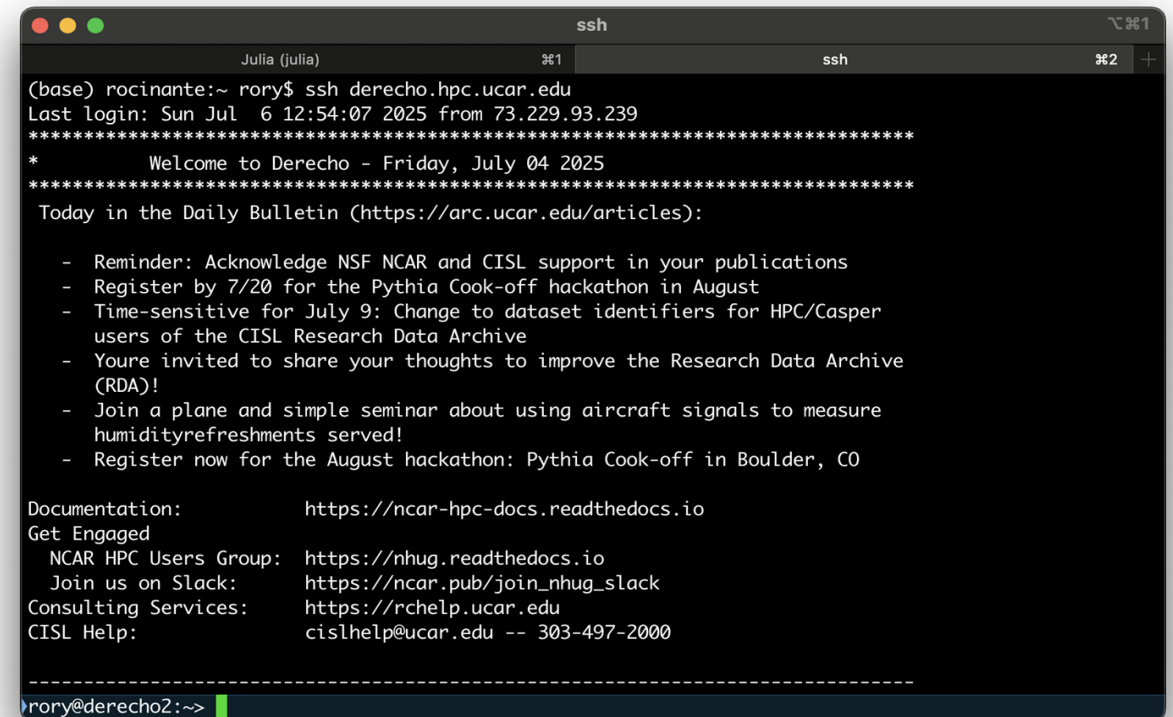
Some of you may not have - ask an assistant during the break or the start of the lab section

Once Duo is set up, authentication occurs in two stages

- 1) Enter a password
- 2) Wait for a push notification and respond

System Access - Logging in from a Terminal

- Use ssh along with your username to log in
ssh -l username derecho.hpc.ucar.edu
ssh username@derecho.hpc.ucar.edu
ssh -l username casper.hpc.ucar.edu
ssh username@caser.hpc.ucar.edu
- Use Duo for authentication
- Derecho - 8 login nodes
- Casper - 2 login nodes



```
ssh
Julia (julia) %1 ssh
ssh %2 +
(base) rocinante:~ rory$ ssh derecho.hpc.ucar.edu
Last login: Sun Jul 6 12:54:07 2025 from 73.229.93.239
*****
*      Welcome to Derecho - Friday, July 04 2025
*****
Today in the Daily Bulletin (https://arc.ucar.edu/articles):

- Reminder: Acknowledge NSF NCAR and CISL support in your publications
- Register by 7/20 for the Pythia Cook-off hackathon in August
- Time-sensitive for July 9: Change to dataset identifiers for HPC/Casper
  users of the CISL Research Data Archive
- You're invited to share your thoughts to improve the Research Data Archive
  (RDA)!
- Join a plane and simple seminar about using aircraft signals to measure
  humidityrefreshments served!
- Register now for the August hackathon: Pythia Cook-off in Boulder, CO

Documentation:      https://ncar-hpc-docs.readthedocs.io
Get Engaged
  NCAR HPC Users Group: https://nhug.readthedocs.io
  Join us on Slack:    https://ncar.pub/join\_nhug\_slack
Consulting Services: https://rchelp.ucar.edu
CISL Help:          cislhelp@ucar.edu -- 303-497-2000

-----
rory@derecho2:~>
```

System Access - Duo Authentication

1



2



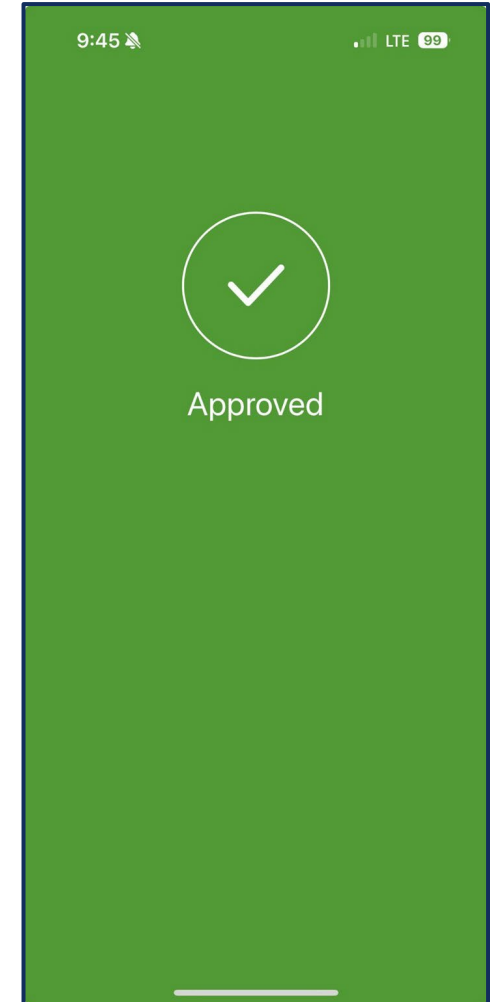
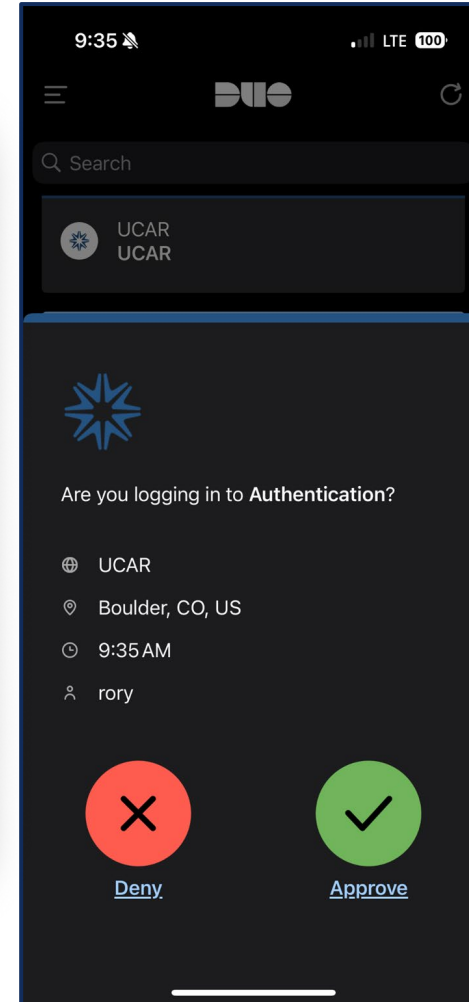
3

```
ssh
Julia (Julia) %1 ssh %2 -bash %3 -bash %4 +
(base) rocinante:~ rory$ ssh rory@derecho.hpc.ucar.edu
Access to and use of this UCAR computer system is limited to authorized use by
UCAR Policies 1-7 and 3-6 and all applicable federal laws, executive orders,
policies and directives. UCAR computer systems are subject to monitoring at all
times to ensure proper functioning of equipment and systems including security
devices, to prevent unauthorized use and violations of statutes and security
regulations, to deter criminal activity, and for other similar purposes.

Users should be aware that information placed in the system is subject to
monitoring and is not subject to any expectation of privacy. Unauthorized use
or abuse will be dealt with according to UCAR Policy, up to and including
criminal or civil penalties as warranted.

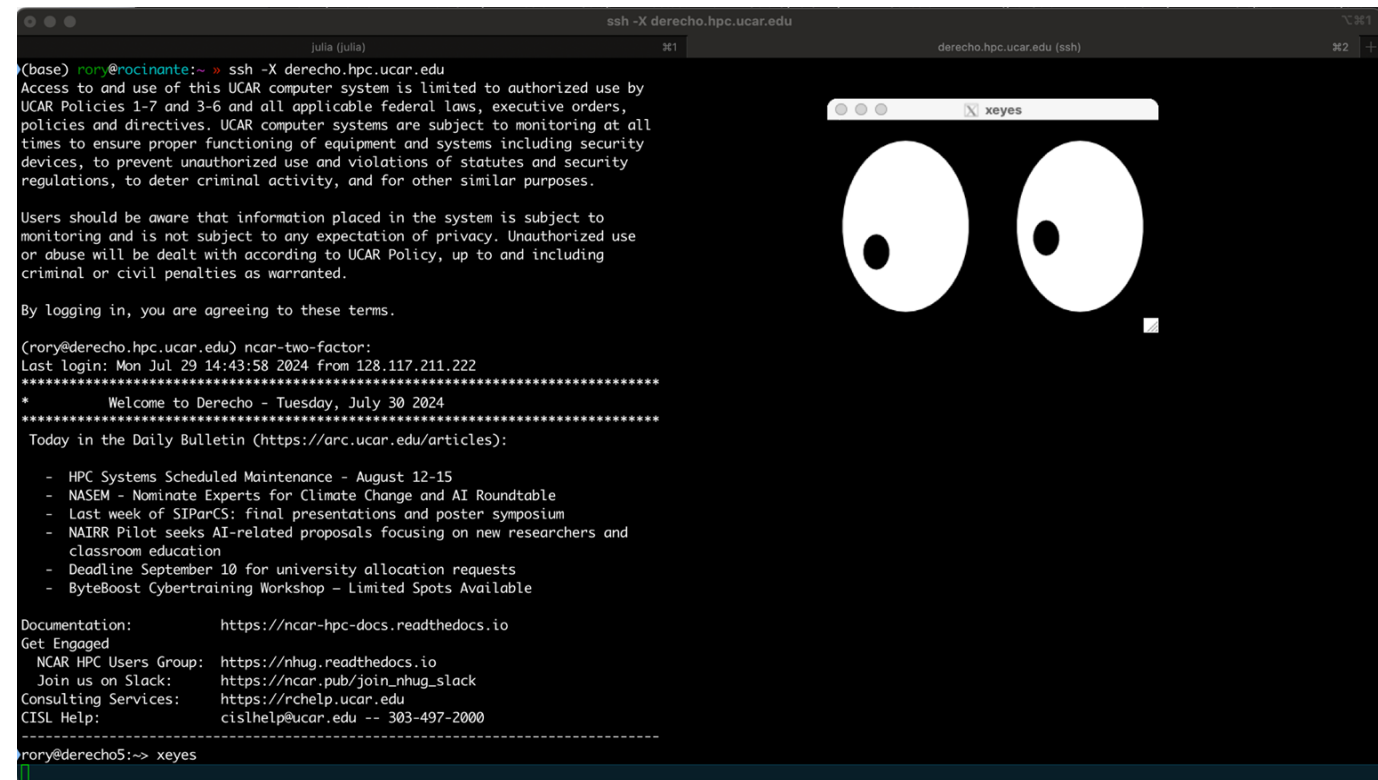
By logging in, you are agreeing to these terms.

(rory@derecho.hpc.ucar.edu) ncar-two-factor:
```



System Access - X11 Forwarding

- Use ssh along with your username to log in
ssh -XY username@derecho 1.hpc.ucar.edu
ssh -XY -l username derecho 1.hpc.ucar.edu
- Use Duo for authentication
- Derecho - 8 login nodes
- Casper - 2 login nodes
- *Basic X11 Forwarding is pretty slow, and not the recommended way to run GUI programs*



```
(base) rory@rocinante:~$ ssh -X derecho.hpc.ucar.edu
Access to and use of this UCAR computer system is limited to authorized use by
UCAR Policies 1-7 and 3-6 and all applicable federal laws, executive orders,
policies and directives. UCAR computer systems are subject to monitoring at all
times to ensure proper functioning of equipment and systems including security
devices, to prevent unauthorized use and violations of statutes and security
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monitoring and is not subject to any expectation of privacy. Unauthorized use
or abuse will be dealt with according to UCAR Policy, up to and including
criminal or civil penalties as warranted.

By logging in, you are agreeing to these terms.

(rory@derecho.hpc.ucar.edu) ncar-two-factor:
Last login: Mon Jul 29 14:43:58 2024 from 128.117.211.222
*****
*      Welcome to Derecho - Tuesday, July 30 2024      *
*****
Today in the Daily Bulletin (https://arc.ucar.edu/articles):

- HPC Systems Scheduled Maintenance - August 12-15
- NASEM - Nominate Experts for Climate Change and AI Roundtable
- Last week of SIPaCIS: final presentations and poster symposium
- NAIRR Pilot seeks AI-related proposals focusing on new researchers and
  classroom education
- Deadline September 10 for university allocation requests
- ByteBoost Cybertraining Workshop - Limited Spots Available

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  Join us on Slack:    https://ncar.pub/join\_nhug\_slack
Consulting Services: https://rhelp.ucar.edu
CISL Help:          cislhelp@ucar.edu -- 303-497-2000
-----
rory@derecho5:~$ xeyes
```

Run GUI Programs with VNC

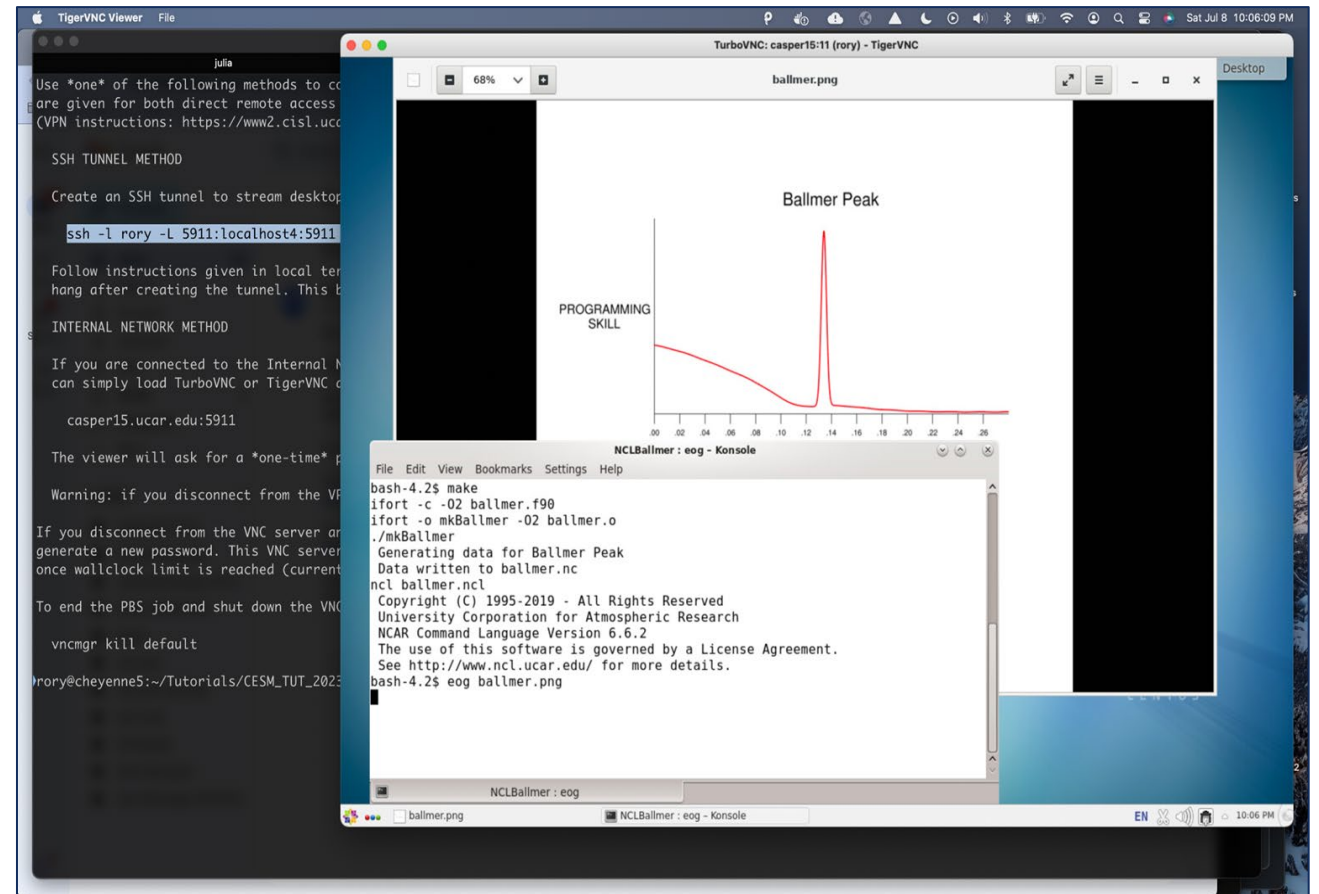
VNC can be used to run a remote GNOME/KDE desktop

Need to install a VNC client first - We recommend TigerVNC, but other VNC clients such as TurboVNC will also work

Usage:

```
vncmgr create -A <project code>
```

```
vncmgr (interactive)
```



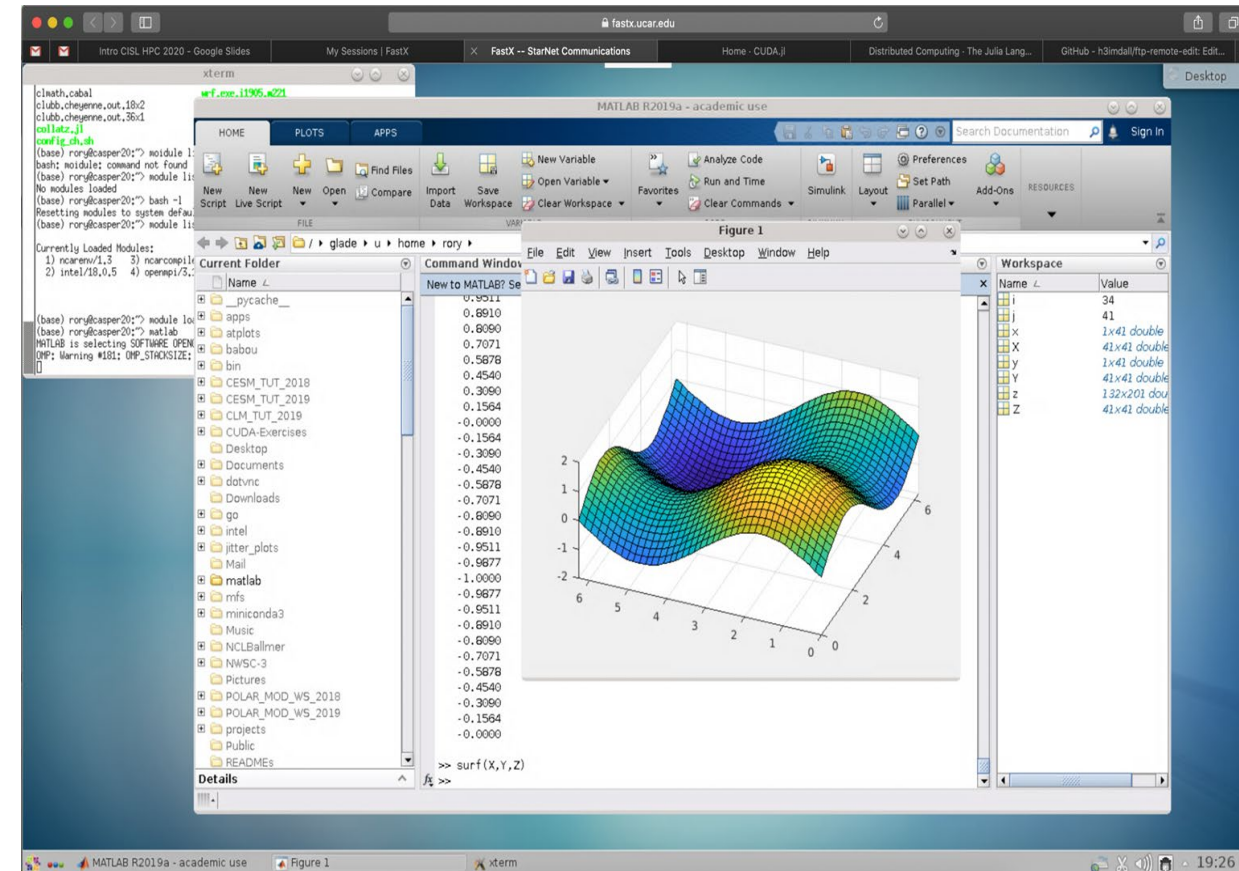
Run GUI Programs with FastX

FastX can be used to run a remote desktop or terminal session in a browser without a client.

Connect to the NCAR VPN, then go to
<https://fastx.ucar.edu:3300>

Can also be setup using an SSH tunnel

- `ssh -L 3300:fastx.ucar.edu:3300`
username@fastx.ucar.edu (duo auth)
- Go to `https://localhost:3300` in a browser
ignore unsafe warnings
duo auth again
- Open a KDE Desktop



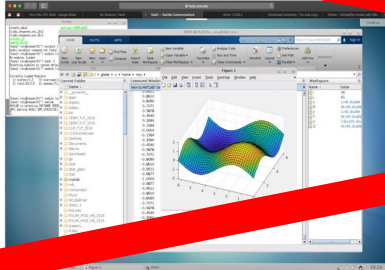
Open OnDemand

GUI Programs with FastX

FastX can be used to run a remote desktop session in a browser without a client.

Connect to the NCAR VPN, then go to <https://fastx.ucar.edu:3300>

- Can also be setup using an SSH tunnel
- `ssh -L 3300:fastx.ucar.edu:3300 username@fastx.ucar.edu` (duo auth)
 - Go to `https://localhost:3300` in a browser
 - ignore unsafe warnings
 - duo auth again
 - Open a KDE Desktop

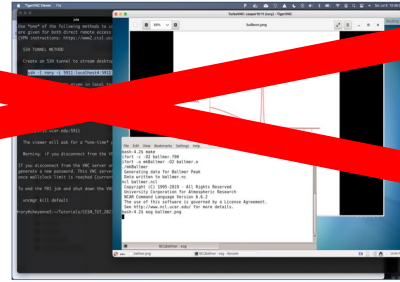


Run GUI Programs with VNC

VNC can be used to run a remote GNOME/KDE desktop

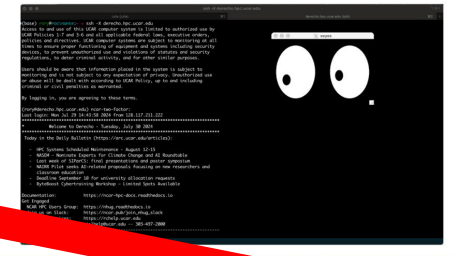
Need to install a VNC client first - We recommend TigerVNC, but other VNC clients such as TurboVNC will also work

Usage:
`vncmgr create -A <sp>`
`vncmgr` (interactive)



System Access - X11 Forwarding

- Use ssh along with your username: `ssh -XY username@hpc.ucar.edu`
- Username: `username` (e.g., `derecho1.hpc.ucar.edu`)
- Use Duo for authentication
- Derecho - 8 login nodes
- Casper - 2 login nodes
- **Basic X11 Forwarding is pretty slow, and not the recommended way to run GUI**

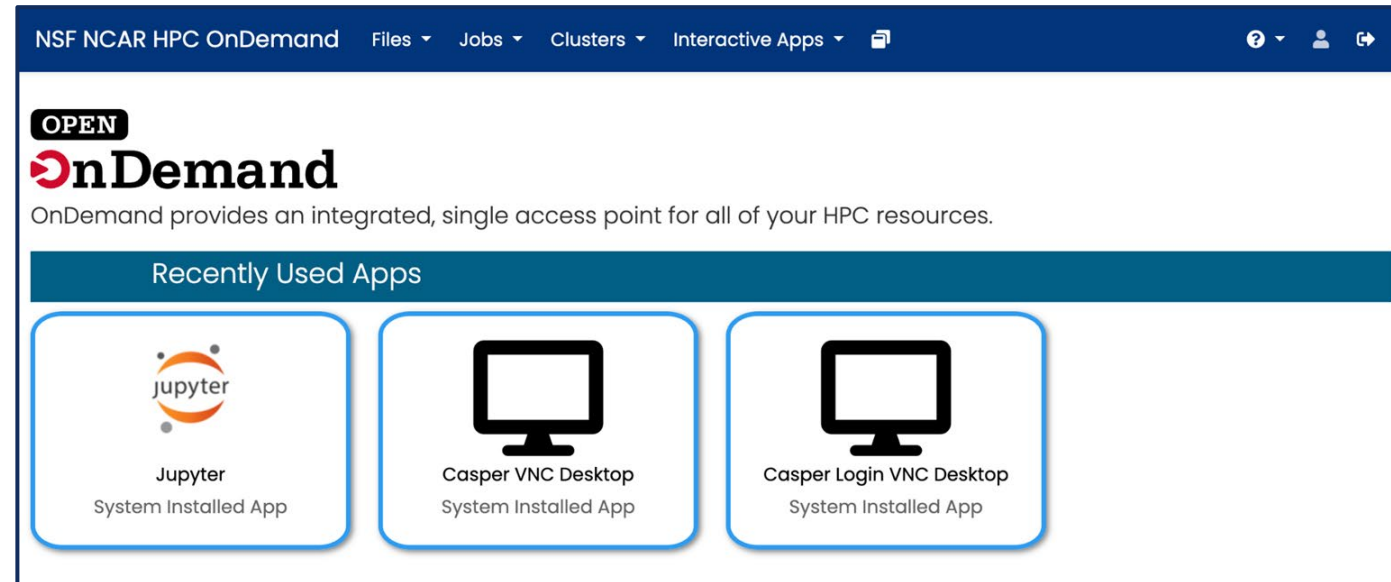
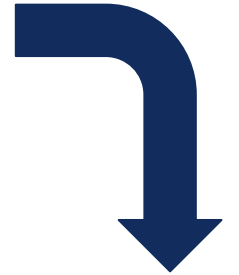
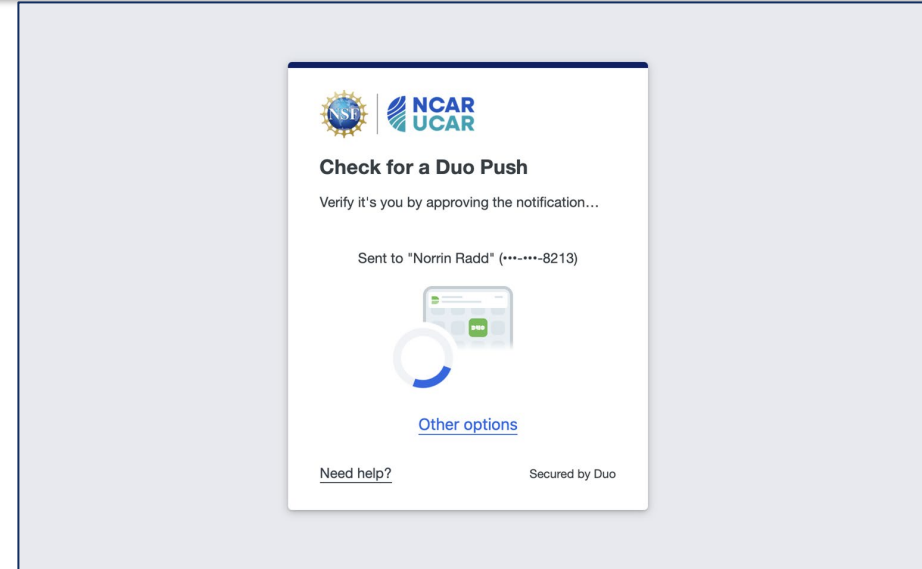
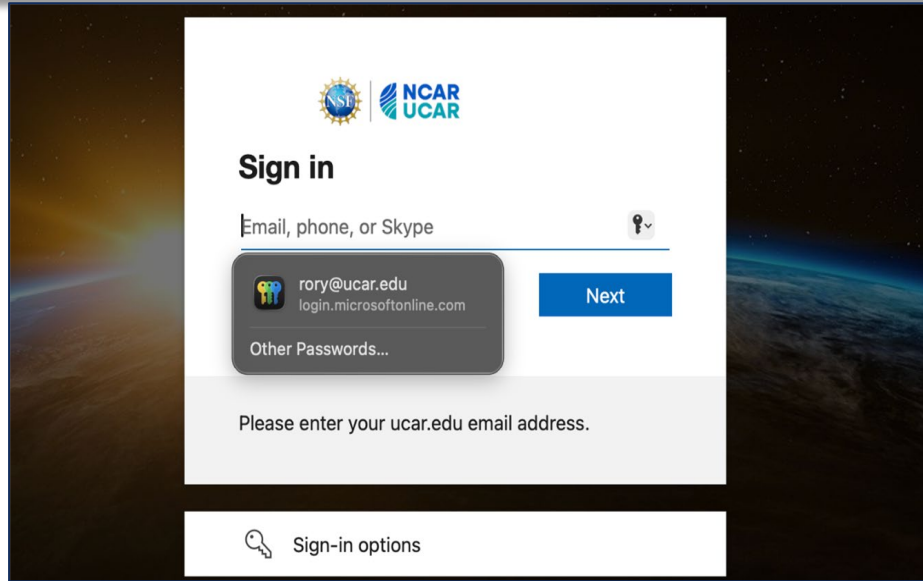


New **Open OnDemand** service can be used as easier method for X11, VNC, and Jupyterhub

- Doesn't require local installation of software
- Authentication via a single Duo authentication step
- VPN access not required

Access in browser at <https://ondemand.hpc.ucar.edu>

Open OnDemand - Logging In



<https://ondemand.hpc.ucar.edu>
Log in with your standard Duo credentials and respond to the push notification

Open OnDemand - Landing Page

NSF NCAR HPC OnDemand

Files ▾

Jobs ▾

Clusters ▾

Interactive Apps ▾



OPEN

OnDemand

OnDemand provides an integrated, single access point for all of your HPC resources.

Recently Used Apps



Jupyter

System Installed App



Casper VNC Desktop

System Installed App



Casper Login VNC Desktop

System Installed App



Open OnDemand - Landing Page

NSF NCAR HPC OnDemand

Files ▾

Jobs ▾

Clusters ▾

Interactive Apps ▾



OPEN

OnDemand

OnDemand provides an integrated, single access point

Recently Used Apps



Jupyter

System Installed App



Casper VNC Desktop

System Installed App



Casper Login VNC Desktop

System Installed App

Desktops

🖥️ Casper Login VNC Desktop

🖥️ Casper VNC Desktop

GUIs

🔥 MATLAB

Servers

📄 Code Server

🔥 Jupyter



Open OnDemand - Jupyterhub

The screenshot shows the NSF NCAR HPC OnDemand web interface. The top navigation bar includes links for Files, Jobs, Clusters, and Interactive Apps. The breadcrumb trail indicates the user is in the Jupyter section. A left sidebar lists various interactive applications, with Jupyter selected. The main content area for Jupyter provides instructions to launch a server with Python on the Casper cluster. Below this, there are four dropdown menus for configuration: Cluster (set to Casper), Resource Selection (set to Casper PBS batch), Queue or Reservation (-q) (set to casper), and Project Account (-A) (set to SSSG0001). A note at the bottom of the configuration section asks the user to select the account to charge for the job.

NSF NCAR HPC OnDemand Files Jobs Clusters Interactive Apps

Home / My Interactive Sessions / Jupyter

Interactive Apps

- Desktops
 - Casper Login VNC Desktop
 - Casper VNC Desktop
- GUIs
 - MATLAB
- Servers
 - Code Server
 - Jupyter**

Jupyter

Launch a [Jupyter](#) server with [Python](#) on the Casper cluster. Check the [Changelog](#) for the recent updates.

Cluster

Casper

Resource Selection

Casper PBS batch

Queue or Reservation (-q)

casper

Project Account (-A)

SSSG0001

Select the account to charge for this job.

Select a Resource and fill in batch details, including number of cores and project account

Open OnDemand - Jupyterhub

Specify Memory per Node in GB (-l mem=N)

Specify X Number of GPUs / Node (-l ngpus=X)

Select GPU Type, X (-l gpu_type=X)

Wall Time in hours (24-hour max)

Jupyter Environment

☐ I would like to receive an email when the session starts

Launch

* The Jupyter session data for this session can be accessed under the [data root directory](#).

After selecting resources
click “Launch” to start
the jupyterhub session

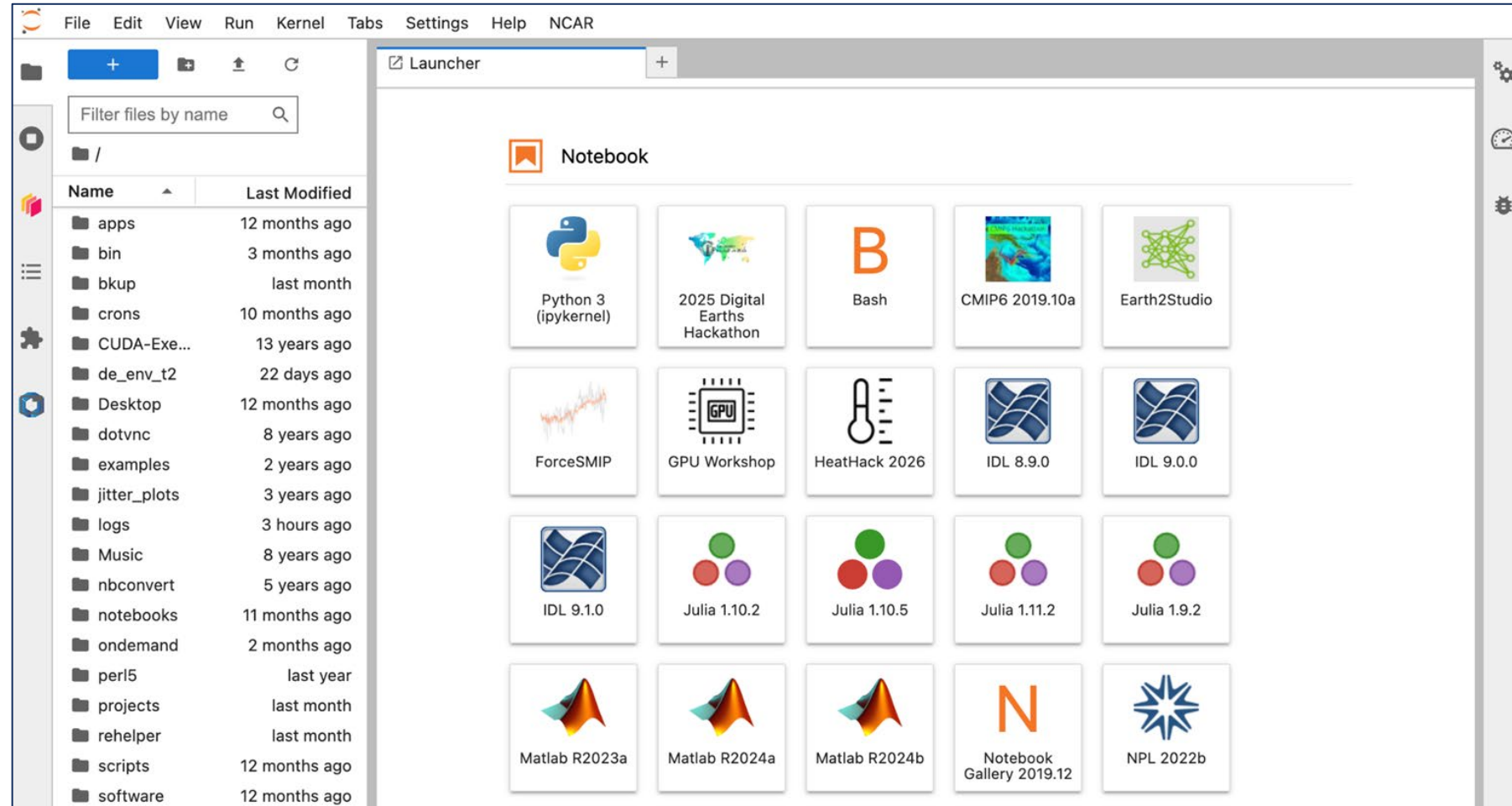
Open OnDemand - Jupyterhub

The screenshot displays the NSF NCAR HPC OnDemand web interface. At the top, a dark blue navigation bar contains the text "NSF NCAR HPC OnDemand" and several menu items: "Files", "Jobs", "Clusters", and "Interactive Apps". To the right of these menus are icons for help, user profile, and sharing. Below the navigation bar, a green notification box states "Session was successfully created." with a close button. A breadcrumb trail shows "Home / My Interactive Sessions". On the left, a sidebar titled "Interactive Apps" lists categories: "Desktops" (Casper Login VNC Desktop, Casper VNC Desktop), "GUIs" (MATLAB), and "Servers" (Code Server, Jupyter). The main content area features a green header for a Jupyter session: "Jupyter (5059307.casper-pbs)" with status indicators "1 node | 1 core | Running". Below this, the "Host" is shown as a terminal icon followed by "crhte70.hpc.ucar.edu", and a red "Delete" button is present. The "Created at" timestamp is "2026-07-01 21:36:12 MDT", and the "Time Remaining" is "59 minutes". The "Session ID" is "2ec37c5b-1bd8-4226-a2a5-a2b9dbe2271d". At the bottom of the session card is a blue button labeled "Connect to Jupyter" with a gear icon.

Once resources are ready you are able to connect to the jupyter session

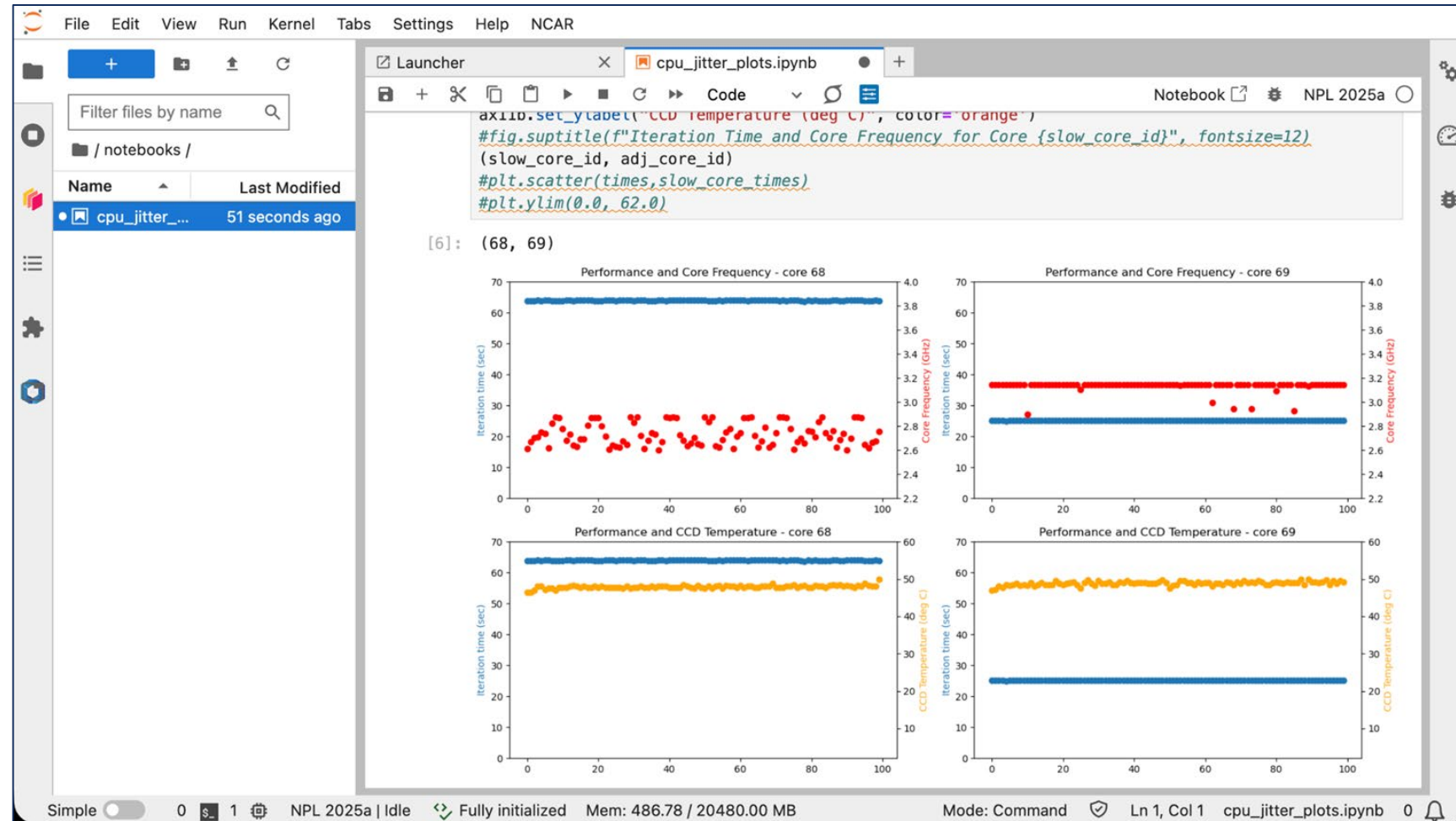
Open OnDemand - Jupyterhub

Many Notebooks and applications can be run from the main jupyterhub launcher screen.



Open OnDemand - Jupyterhub

Jupyterhub is useful for creating sophisticated interactive notebooks for analysis, education, etc.



Open OnDemand - VNC Sessions

Open OnDemand is also very useful for running Desktop VNC sessions from the browser

The screenshot displays the NSF NCAR HPC OnDemand web interface. At the top, a dark blue navigation bar contains the text "NSF NCAR HPC OnDemand" and several menu items: "Files", "Jobs", "Clusters", "Interactive Apps", and "My Interactive Sessions". On the right side of the bar are links for "Help", "Logged in as rory", and "Log Out".

Below the navigation bar, a green notification box states "Session was successfully deleted." with a close button. A breadcrumb trail shows "Home / My Interactive Sessions".

The main content area is divided into two sections. On the left, a sidebar titled "Interactive Apps" lists categories: "Desktops" (with "Casper Login VNC Desktop" and "Casper VNC Desktop"), "GUIs" (with "MATLAB"), and "Servers" (with "Code Server" and "Jupyter").

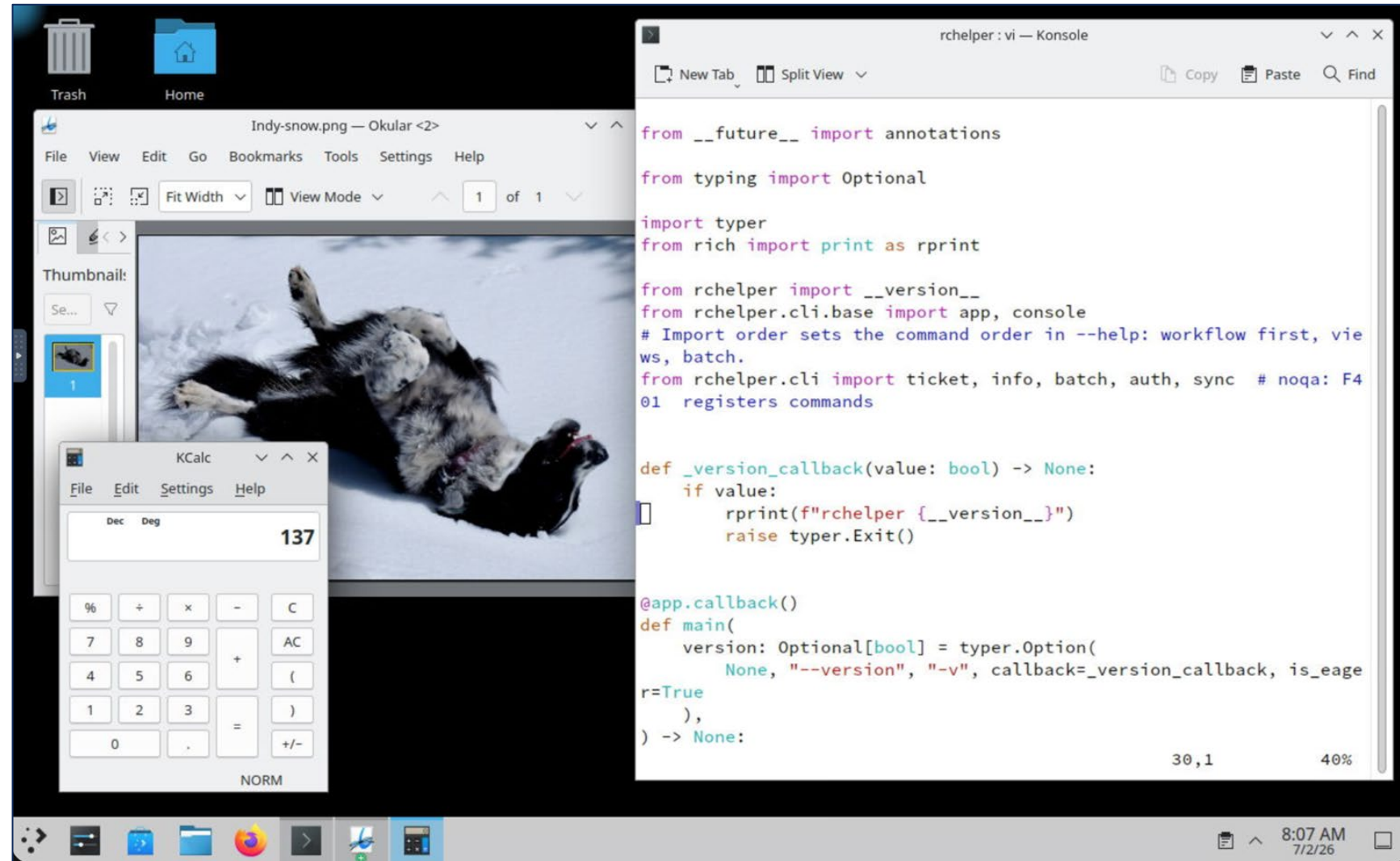
The right section features a card for a "Casper VNC Desktop (5060236.casper-pbs)" session. The card has a green header with "1 node | 1 core | Running". It includes a "Host" field with a dropdown menu showing "casper45.hpc.ucar.edu", a "Delete" button, and a "Created at" timestamp of "2026-07-02 07:35:22 MDT". Below this, it shows "Time Remaining: 45 minutes" and a "Session ID: ad6a85fd-flaa-4c22-a227-2d2eca63ae36".

At the bottom of the card, there are two sliders: "Compression" (ranging from 1 (low) to 9 (high)) and "Image Quality" (ranging from 0 (low) to 9 (high)). A "Launch Casper VNC Desktop" button is positioned below the sliders, and a "View Only (Share-able Link)" button is on the right.

Open OnDemand - VNC Sessions

A VNC Desktop session gives you a virtual Linux Desktop on Casper from your browser

X11 is automatically enabled from within a VNC Desktop session



Be a Good Neighbor on Shared Resources

- Your activities coexists with those of other users
- CPUs and memory are shared on the login nodes
- Limit your usage to:
 - Reading and editing text/code
 - Compiling small programs
 - Performing data transfers
 - Interacting with the job scheduler
- Programs that use excessive resources on the login nodes will be limited (you will receive automated warnings via email if you exceed usage thresholds)
- In extreme cases, your processes may be terminated

Data Storage - GLADE

File spaces accessible from all HPC systems

File space	Quota	Backup	Uses
Home /glade/u/home/\$USER	50 GB	Yes	Settings, code, scripts
Work /glade/work/\$USER	2 TB	No	Compiled codes, models
Scratch /glade/derecho/scratch/\$USER	30 TB	Purged!	Run directories, temp output
Campaign /glade/campaign	N/A	No	Project space allocations

*Keep track of usage with “**gladequota**”*



Moving data to and from GLADE

- For short transfers use **scp/sftp** to transfer files
- For large transfers use **Globus**
 - To use Globus, create a Globus ID if you need an account, and search for **NCAR GLADE** or **NCAR Campaign Storage** endpoints
 - CISL endpoints currently can be activated for up to 30 -days
 - Globus has a web interface and a command -line interface
 - **Globus Connect Personal** can manage transfers from your local workstation as well

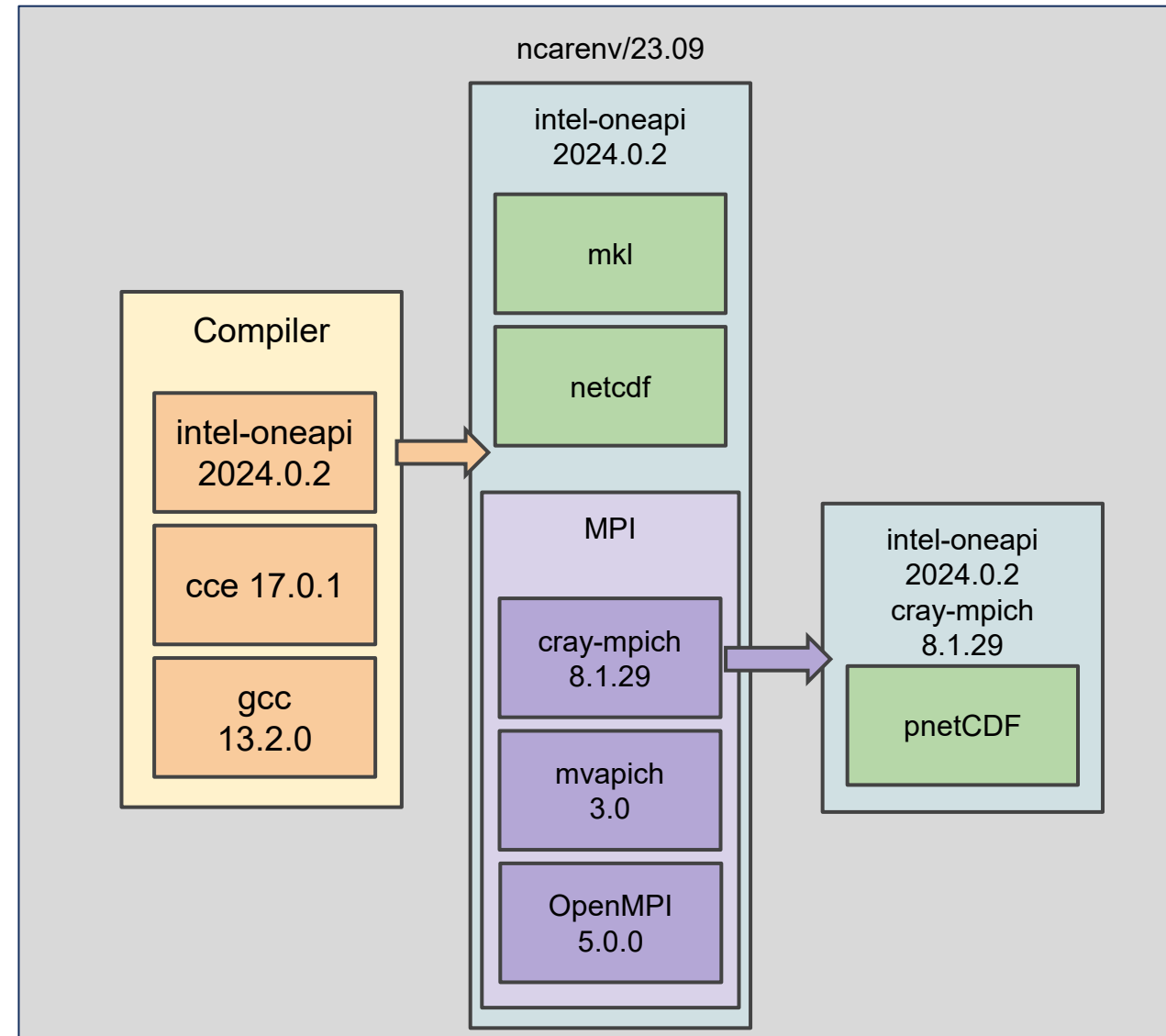


Environment Modules

- CISL installed software is provided as modules
- Modules provide access to runnable applications (compilers, debuggers, ...) as well as libraries (NetCDF, MPI, ...)
- Modules help ensure that all the software in your environment is mutually compatible
- **Note that Derecho and Casper each have independent collections of modules due to differences in their base software stacks. We make an effort to keep the stacks similar, but it is not possible in all cases.**

Using Modules

- **module load/unload <software>**
- **module avail**
 - show all currently-loadable modules
- **module list**
 - show loaded modules
- **module (--force) purge**
 - remove all loaded modules
- **module save/restore <name>**
 - create/load a saved software set
- **module spider <software>**
 - search for a particular module

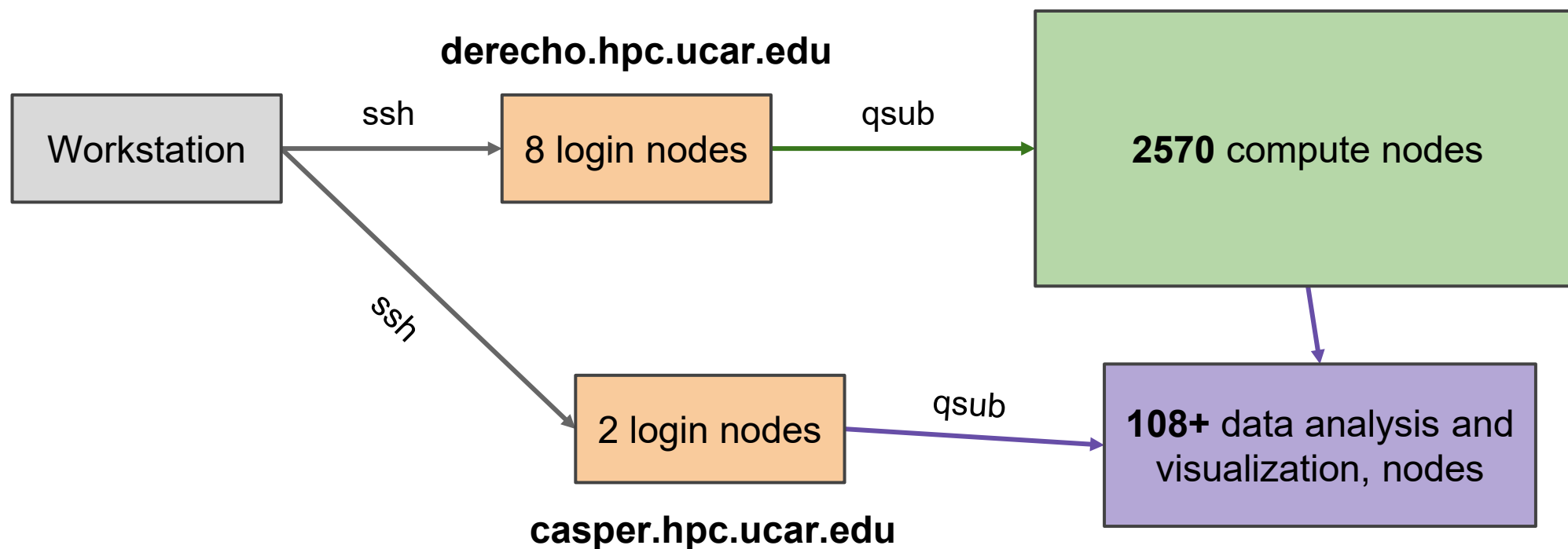


Available Software

- Compilers (Intel, CCE, GCC, NVHPC)
- Debuggers / Performance Tools (Linaro Forge, DDT, MAP, CrayPAT)
- MPI Libraries (Cray-MPICH, MVAPICH*, OpenMPI*, IntelMPI*)
- IO Libraries (NetCDF, PNetCDF, HDF5, Parallel IO)
- Analysis Languages (Python, Julia, R, IDL, Matlab)
- Convenience Tools (ncarccompilers, mpibind, parallel, rclone)
- Many more ...

Using Batch Jobs and Compute Nodes

- Most tasks require too many resources to run on a login node
- Schedule these tasks to run on compute nodes using the **PBS** batch system



Derecho and Casper use separate allocations!

Using Batch Jobs and Compute Nodes

- Jobs request a given amount of compute resources, for an estimated amount of time, on specific hardware
- Jobs use core-hours, which are charged against your selected project/account
 - Remaining resources are viewable in SAM (sam.ucar.edu)
- Temporary files are often written by programs - set TMPDIR variable to scratch space to avoid job failures

Interacting with the PBS Scheduler

qsub <script> - submit batch job

qstat <jobid> - query job status

qdel <jobid> - delete/kill a job

qinteractive -A <project>

Run an interactive job

qcmd -A <project> -- <command>

Run a heavy-weight command on a compute node

Example PBS Batch Script

```
$ cat basic_mpi.pbs
#!/bin/bash
#PBS -N hello_pbs
#PBS -A <project_code>
#PBS -j oe
#PBS -k eod
#PBS -q main
#PBS -l walltime=00:05:00
#PBS -l select=8:ncpus=128:mpiprocs=128

### Set temp to scratch
export TMPDIR=/glade/derecho/scratch/${USER}/tmp
mkdir -p $TMPDIR

module --force purge
module load ncarenv/23.09 intel-oneapi/2024.0.2 ncarcompilers/1.0.0 cray-mpich/8.1.27

### Run MPT MPI Program
mpibind ./hello_world
```

Customize Your Environment with Default Modules

- If you commonly load certain modules, you may wish to have them load automatically when logging onto a cluster
- The right way to do so is with saved module sets:
module --force purge
module load ncarenv/23.09 intel-oneapi/2024.0.2
module load ncarcompilers/1.0.0 cray-mpich/8.1.27
module load conda/latest
module save default
- Make multiple sets and load them using **module restore <set>**
- **Don't put module load commands in your shell startup files!**

Getting Help

HPC Documentation - <https://ncar-hpc-docs.readthedocs.io>

The screenshot shows the NCAR HPC Documentation website. The header includes the NSF and NCAR logos, the title 'NCAR HPC Documentation', a search bar, and a GitHub link. The left sidebar lists navigation options under 'Getting Started' and 'Getting Help'. The main content area features the NCAR Computational & Information Systems Lab logo, a title 'User Documentation for NSF NCAR High Performance Computing', and a paragraph about the documentation's scope. Below this is a 'Selected Links' section with a list of links. Three red arrows point from text labels to specific links: 'Consultant on Duty' points to 'Getting Help', 'Submit a ticket' points to 'NCAR Research Computing', and 'Password Help' points to 'Password Help'.

NCAR HPC Documentation

Getting Started

- End User Agreement
- Accounts >
- Allocations >
- VPN access
- System Usage Policies
- Data Retention Policies
- Best Practices for Supercomputer Users
- Acknowledging NCAR and CISL

Getting Help

Compute Systems and Services

- Derecho >
- Casper >
- CIRRUS >
- Open OnDemand >
- JupyterHub >

NCAR | COMPUTATIONAL & INFORMATION SYSTEMS LAB

User Documentation for NSF NCAR High Performance Computing

This is the home of the user documentation for the NSF NCAR high-performance computing (HPC) and storage resources managed by CISL. It includes searchable information specific to HPC resources, storage systems, authentication procedures and others, as well as additional how-to articles and troubleshooting articles.

Selected Links

- [Getting Started](#)
- [Using Derecho](#)
- [Using Casper](#)
- [Using JupyterHub](#)
- [Getting Help](#)

Don't find what you need? Log in here to submit a help request: [NCAR Research Computing](#).
You need a CIT password to submit a request. Call **303-497-2400** if you don't have one.

Page Outline
Selected Links

Consultant on Duty (points to [Getting Help](#))

Submit a ticket (points to [NCAR Research Computing](#))

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