



Introduction to NCAR HPC Resources

2025 CESM Tutorial

Rory Kelly
HPC Consultant

July 7, 2025

Getting Help

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

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CISL

NCAR HPC Documentation

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Contributing to the Documentation

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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](#)

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



Page Outline

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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

- HPC 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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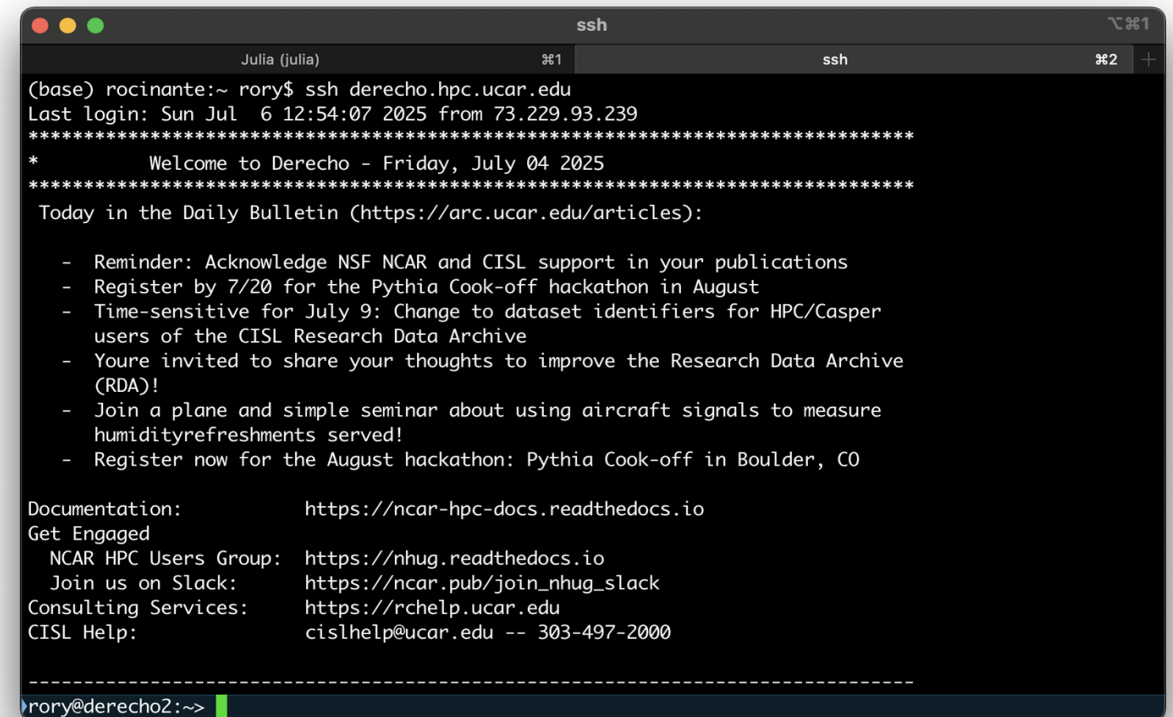
TOO COMPLICATED FOR A SLIDE!

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

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

System Access - 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):

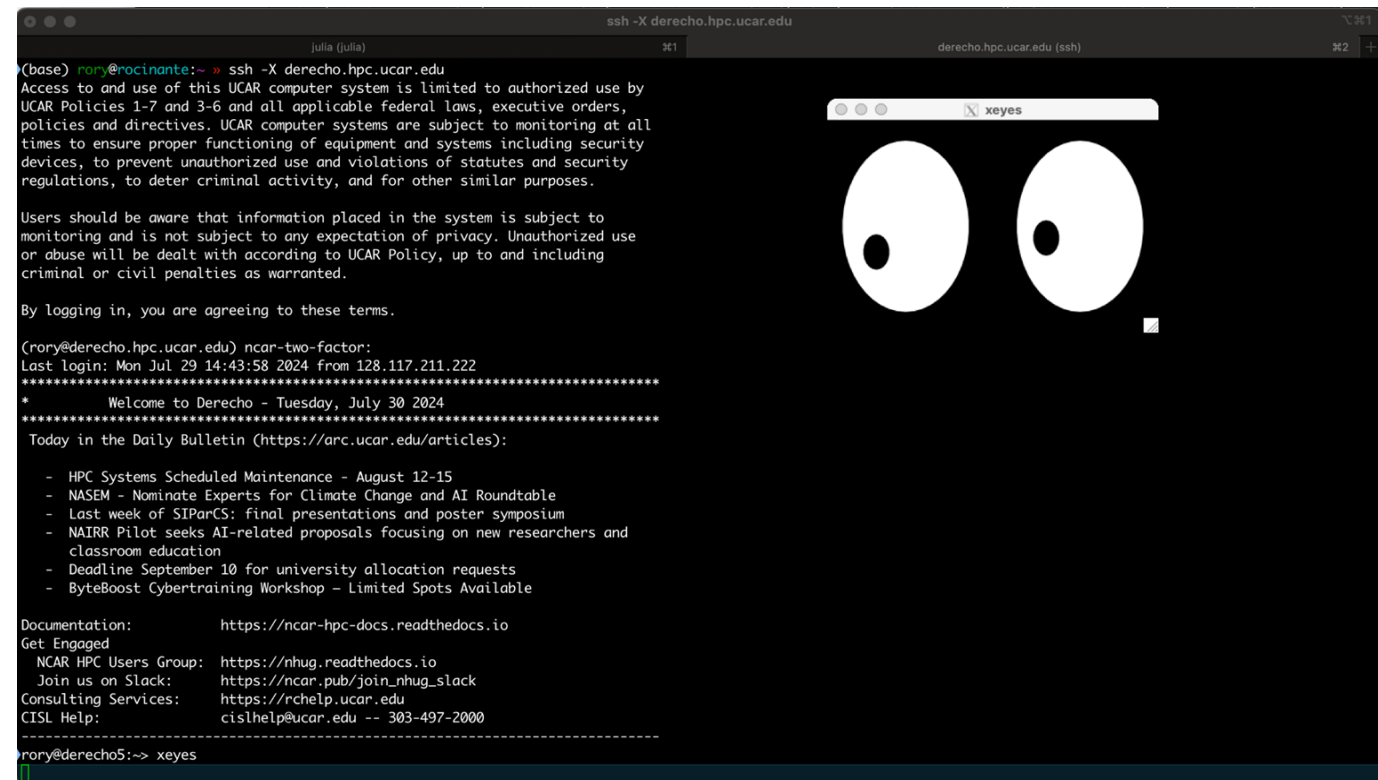
- Reminder: Acknowledge NSF NCAR and CISL support in your publications
- Register by 7/20 for the Pythia Cook-off hackathon in August
- Time-sensitive for July 9: Change to dataset identifiers for HPC/Casper
  users of the CISL Research Data Archive
- You're invited to share your thoughts to improve 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

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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 - X11 Forwarding

- Use ssh along with your username to log in
ssh -XY username@derecho1.hpc.ucar.edu
ssh -XY -l username 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 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
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:
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 SIPaCS: 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

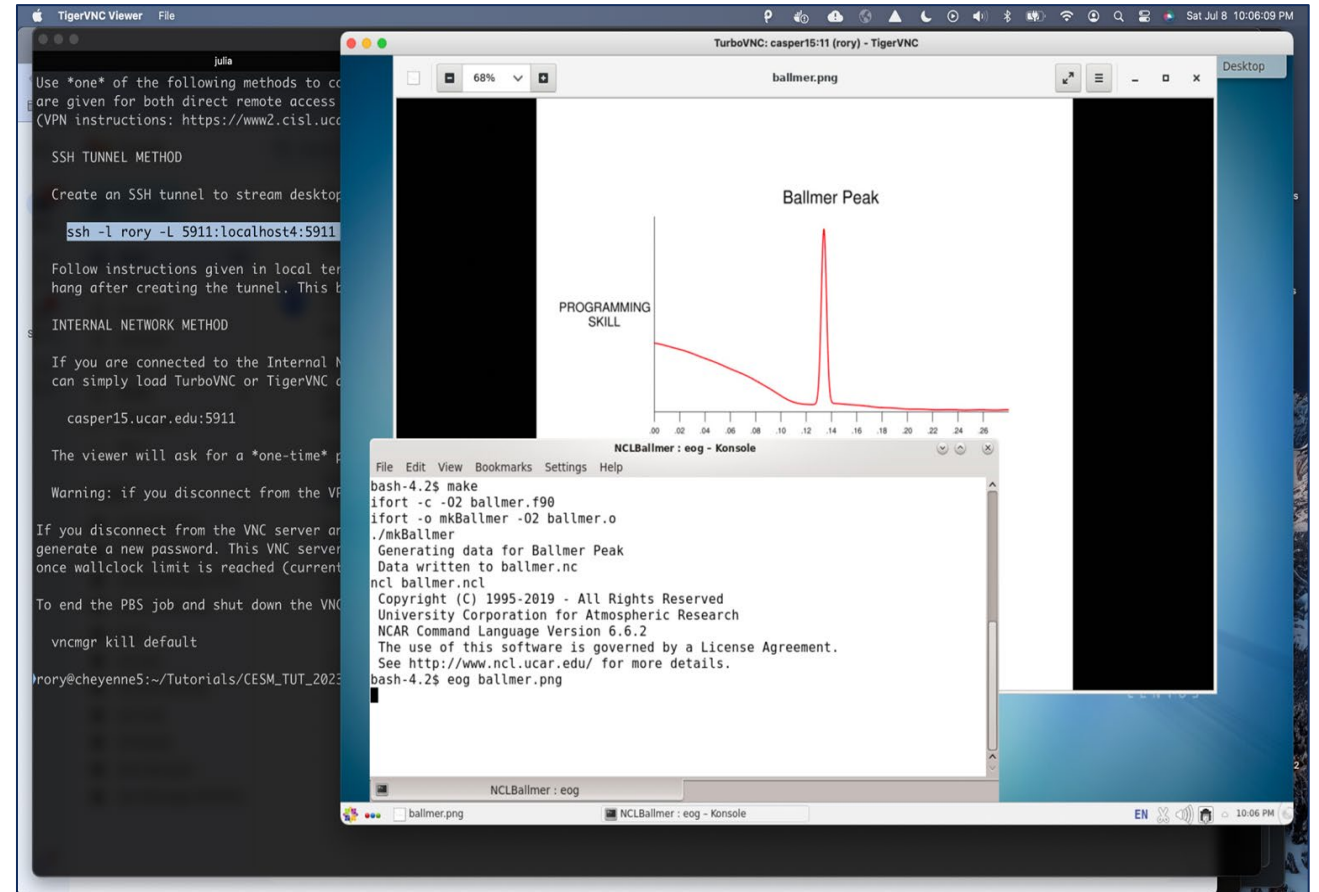
VNC can be used to run a remote GNOME/KDE desktop

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)
```



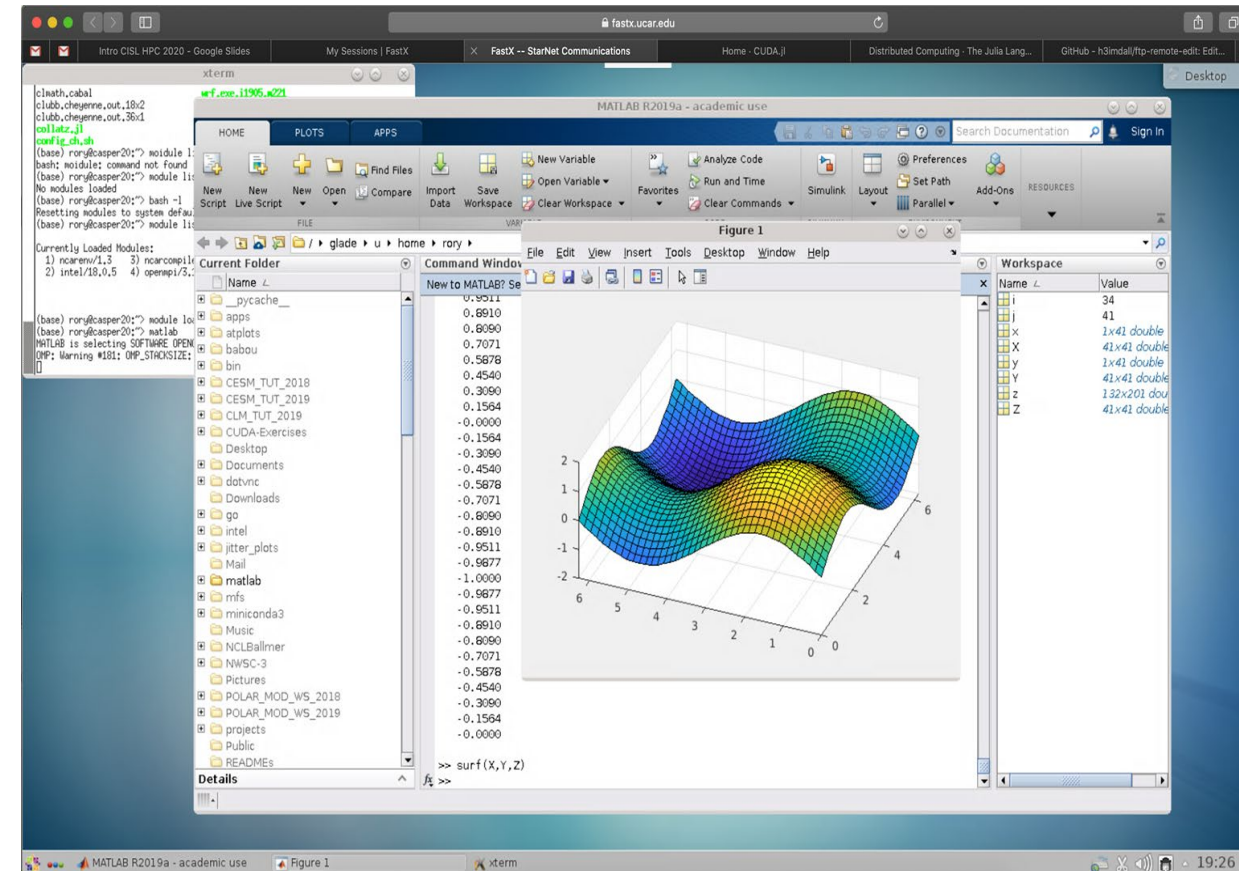
Run GUI Programs with FastX

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>

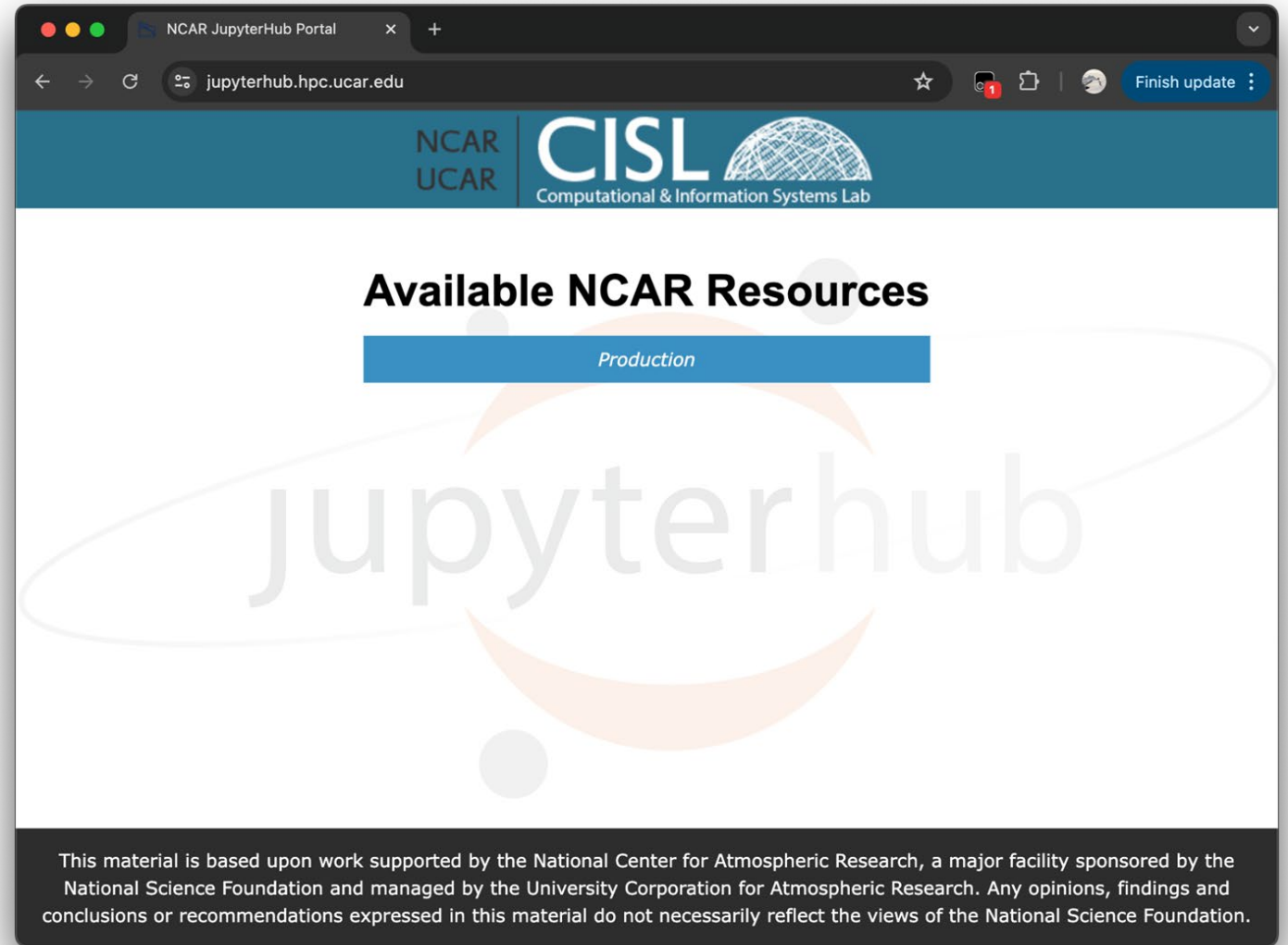
Can also be setup using an SSH tunnel

- `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



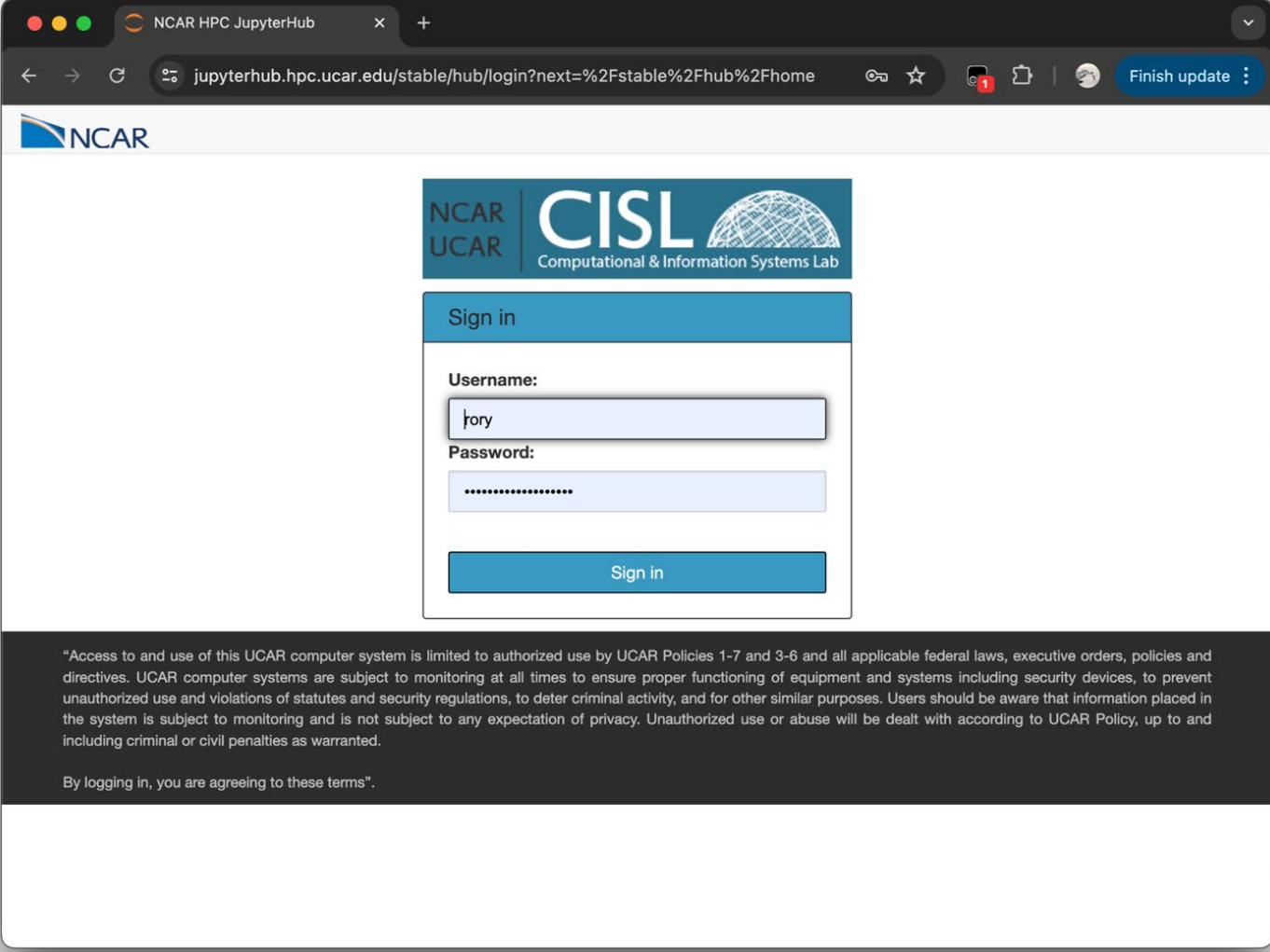
Jupyterhub - Logging In

Derecho and Casper are also accessible via the JupyterHub service at **jupyterhub.hpc.ucar.edu**



Jupyterhub - Logging In

Log in with your standard Duo credentials and respond to the push notification



The screenshot shows a web browser window with the title "NCAR HPC JupyterHub". The address bar shows the URL "jupyterhub.hpc.ucar.edu/stable/hub/login?next=%2Fstable%2Fhub%2Fhome". The page features the NCAR logo in the top left and a header with "NCAR UCAR" and "CISL Computational & Information Systems Lab". The main content area is a "Sign in" form with fields for "Username:" (containing "jory") and "Password:" (masked with dots). A blue "Sign in" button is at the bottom of the form. Below the form, a dark gray footer contains a disclaimer about system access and a statement: "By logging in, you are agreeing to these terms".

NCAR HPC JupyterHub

jupyterhub.hpc.ucar.edu/stable/hub/login?next=%2Fstable%2Fhub%2Fhome

NCAR

NCAR UCAR CISL Computational & Information Systems Lab

Sign in

Username:

jory

Password:

.....

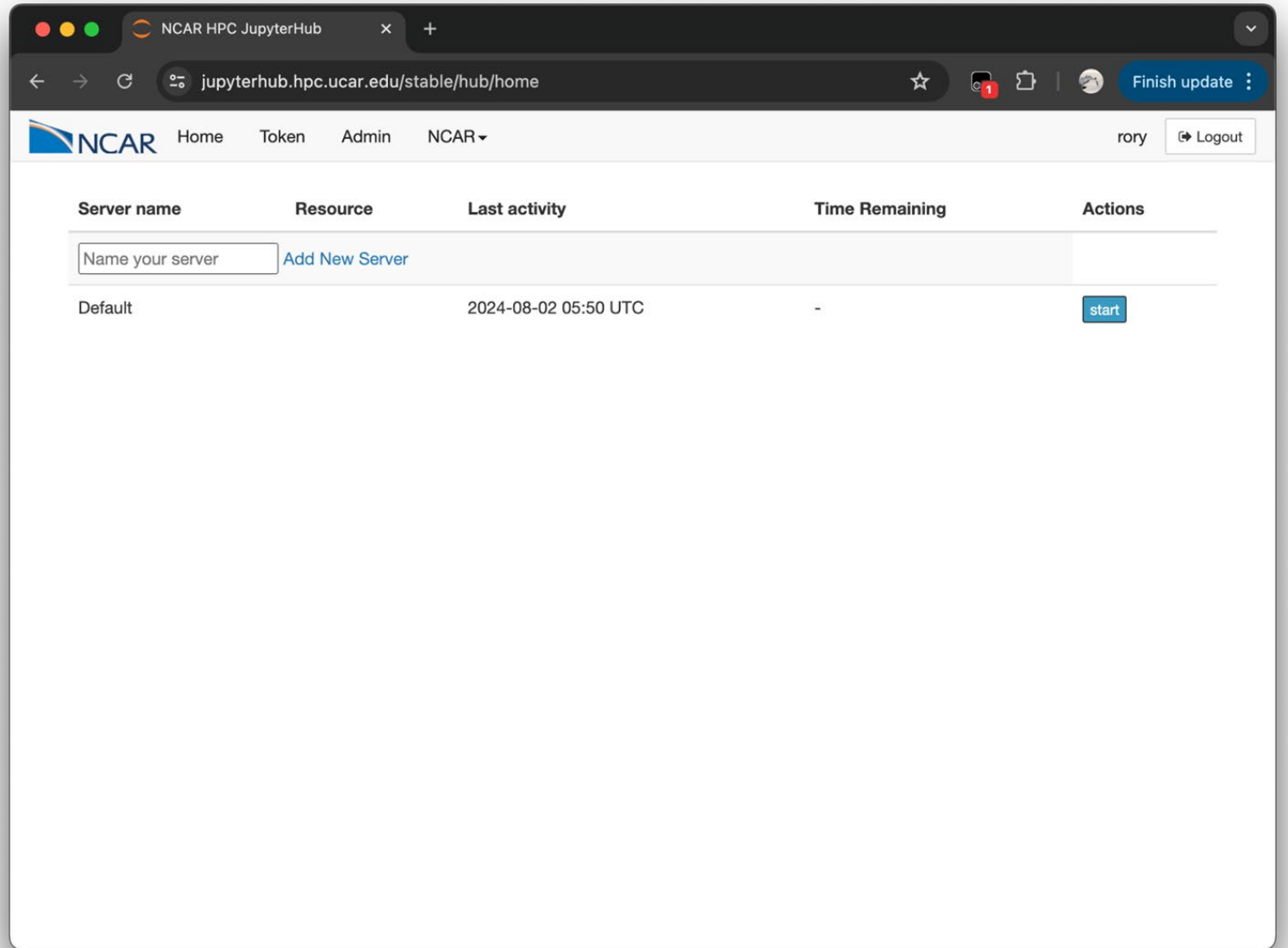
Sign in

"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.

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Jupyterhub - Logging In

Start a server if you do not already have one running

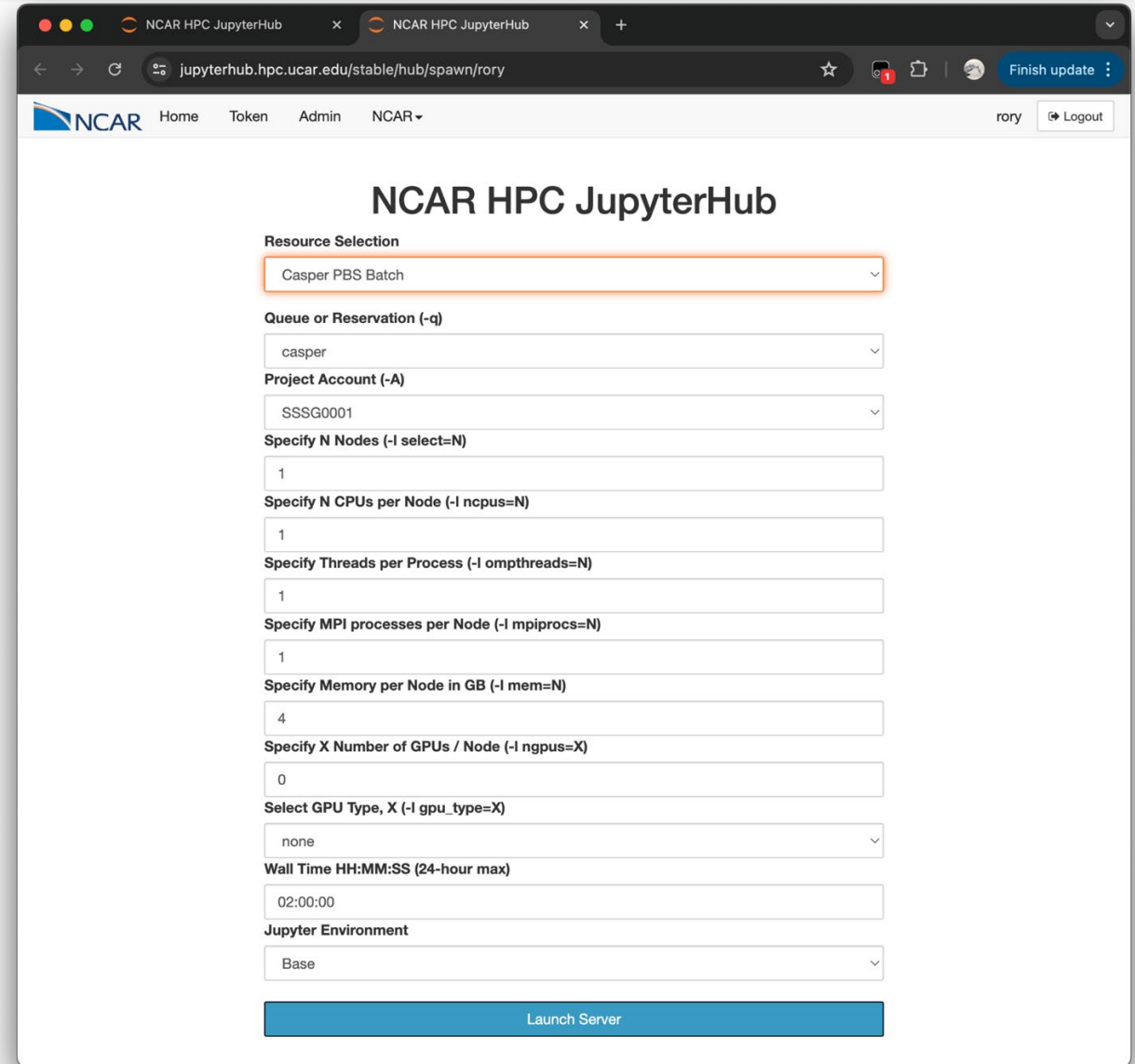


The screenshot shows the NCAR HPC JupyterHub web interface. The browser address bar displays `jupyterhub.hpc.ucar.edu/stable/hub/home`. The page header includes the NCAR logo, navigation links (Home, Token, Admin, NCAR), and a user profile section with the name 'rory' and a 'Logout' button. Below the header is a table with the following columns: 'Server name', 'Resource', 'Last activity', 'Time Remaining', and 'Actions'.

Server name	Resource	Last activity	Time Remaining	Actions
Name your server	Add New Server			
Default		2024-08-02 05:50 UTC	-	start

Jupyterhub - Logging In

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



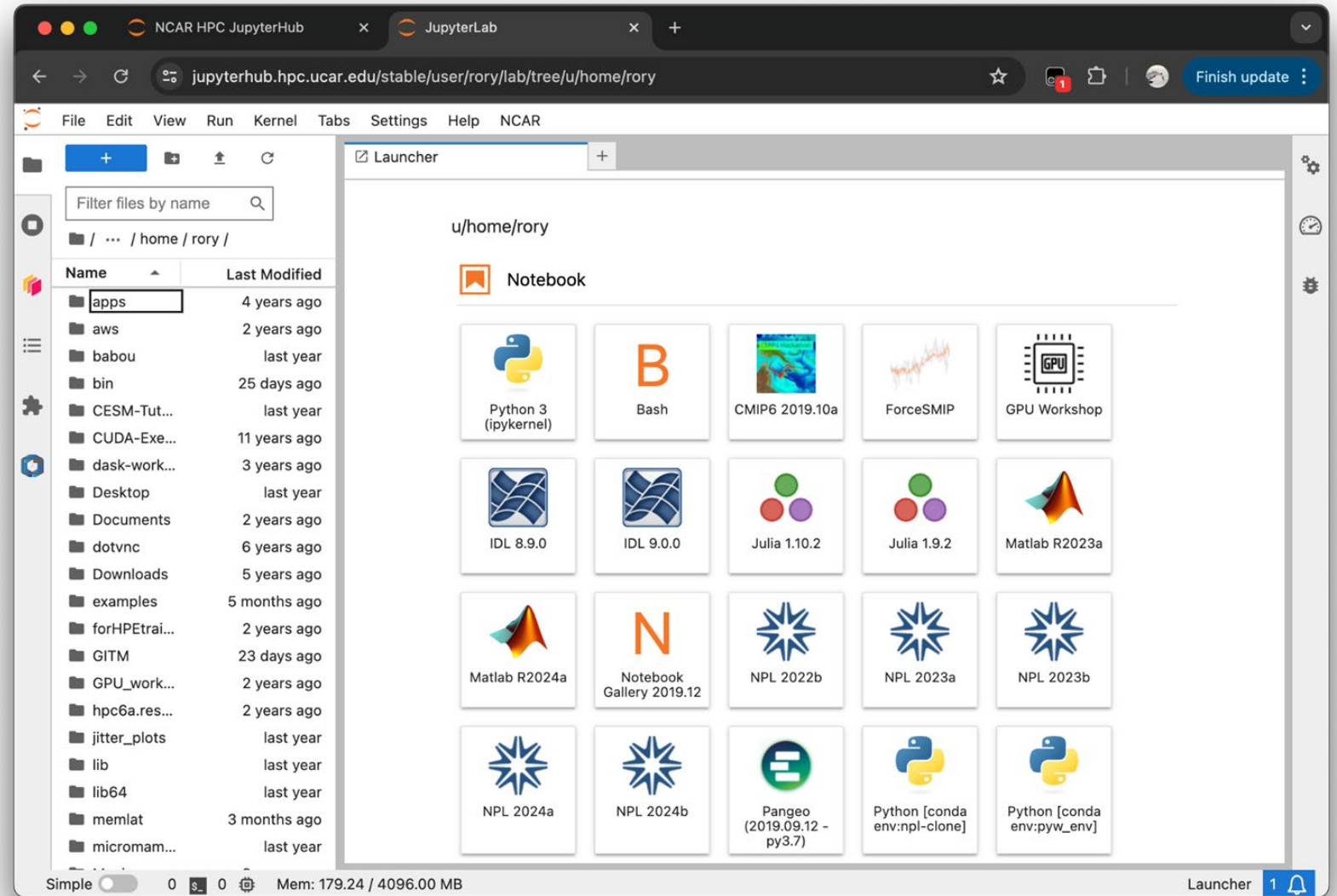
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- Resource Selection:** A dropdown menu with "Casper PBS Batch" selected.
- Queue or Reservation (-q):** A dropdown menu with "casper" selected.
- Project Account (-A):** A dropdown menu with "SSSG0001" selected.
- Specify N Nodes (-l select=N):** A text input field with "1" entered.
- Specify N CPUs per Node (-l ncpus=N):** A text input field with "1" entered.
- Specify Threads per Process (-l ompthreads=N):** A text input field with "1" entered.
- Specify MPI processes per Node (-l mpiprocs=N):** A text input field with "1" entered.
- Specify Memory per Node in GB (-l mem=N):** A text input field with "4" entered.
- Specify X Number of GPUs / Node (-l ngpus=X):** A text input field with "0" entered.
- Select GPU Type, X (-l gpu_type=X):** A dropdown menu with "none" selected.
- Wall Time HH:MM:SS (24-hour max):** A text input field with "02:00:00" entered.
- Jupyter Environment:** A dropdown menu with "Base" selected.

A blue "Launch Server" button is located at the bottom of the form.

Jupyterhub - Logging In

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



Uses for Jupyterhub

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

It can also be used for unsophisticated things like quickly viewing images.



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 <code>/glade/u/home/\$USER</code>	50 GB	Yes	Settings, code, scripts
Work <code>/glade/work/\$USER</code>	2 TB	No	Compiled codes, models
Scratch <code>/glade/derecho/scratch/\$USER</code>	30 TB	Purged!	Run directories, temp output
Campaign <code>/glade/campaign</code>	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

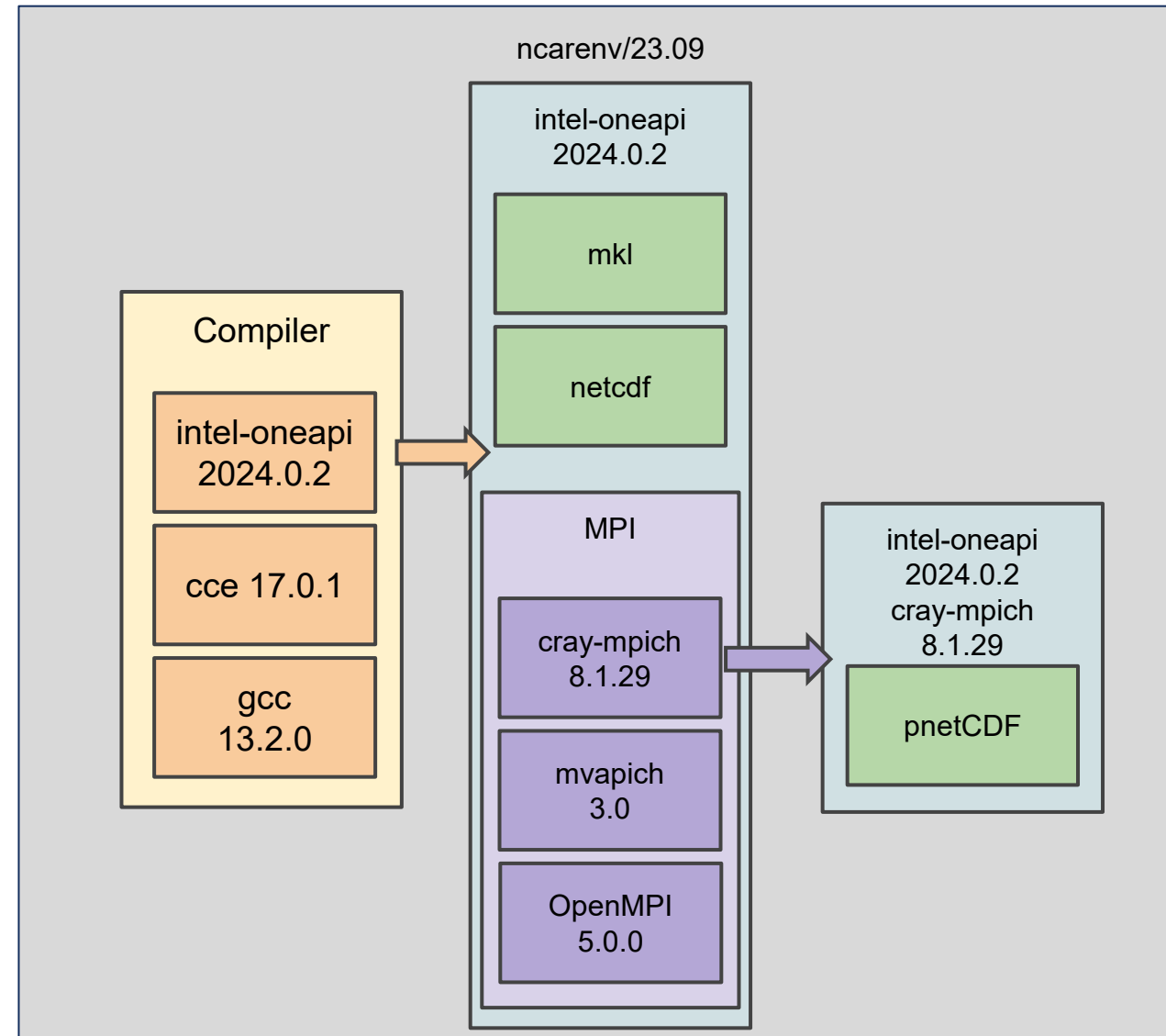


Environment Modules

- 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

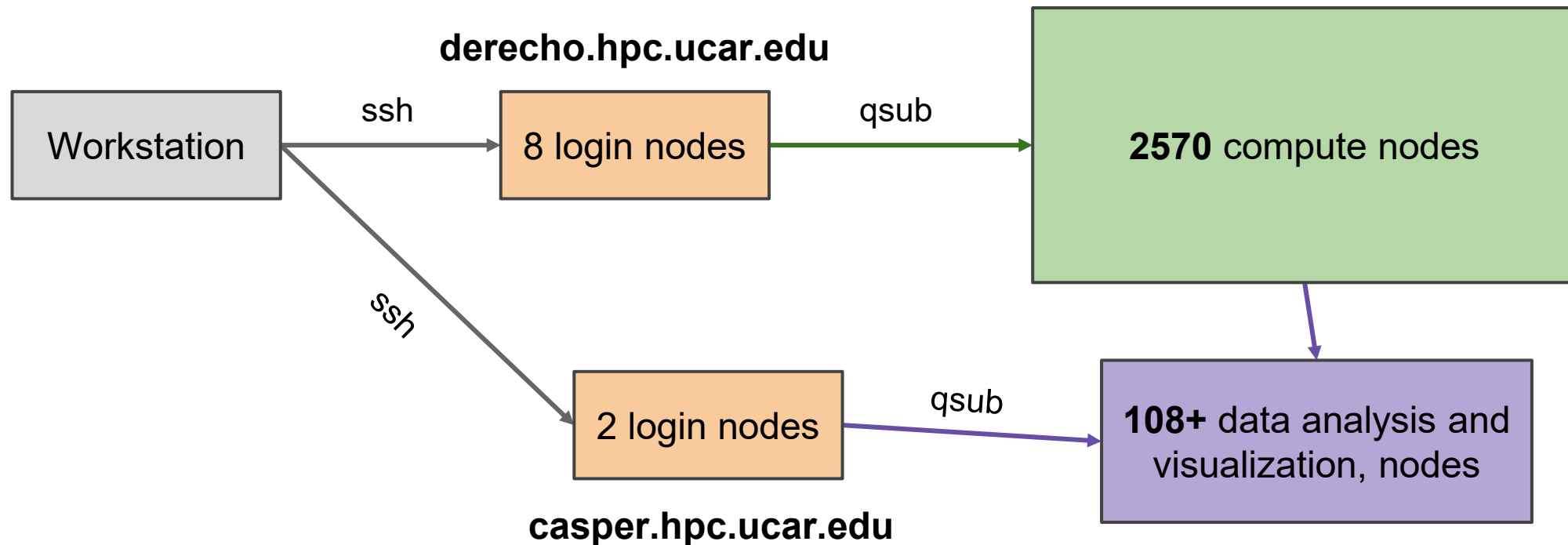


Available Software

- 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!**

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