

What NOT to do!

I love this movie, by the way. This is just NOT how to connect to an HPC resource!













Connecting to NERSC is EASY

What you DO need:

- An internet connection
- a laptop or computer with terminal
- Username, password and Multi-Factor Authentication method







Agenda

Navigating Iris (https://iris.nersc.gov)



- Connecting to Perlmutter
 - a. Connecting with SSH
 - b. https://jupyter.nersc.gov notebooks and terminals in your browser
 - c. NoMachine (https://docs.nersc.gov/connect/nx/) for GUI apps
- Submitting a User Ticket (https://help.nersc.gov)
- Navigating NERSC Documentation
- Navigating NERSC Home Page









What is Iris?

- Lab Notebook for NERSC resource tracking and management
 - Manage password and set up Multi-Factor Authentication
 - Keep track of compute hours, storage space, projects
 - Check compute job history and hours charged
 - and more!

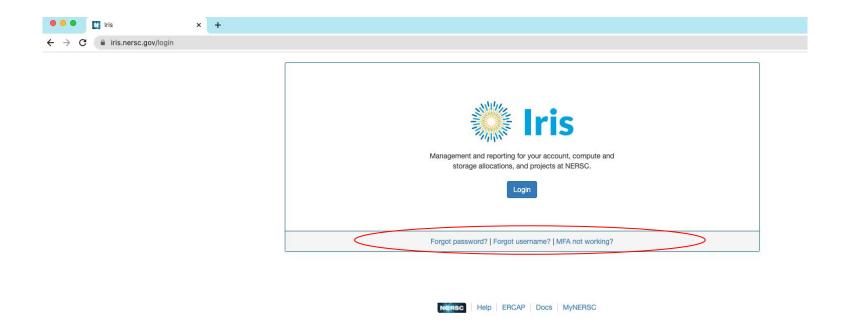








Iris (https://iris.nersc.gov) for Your Account

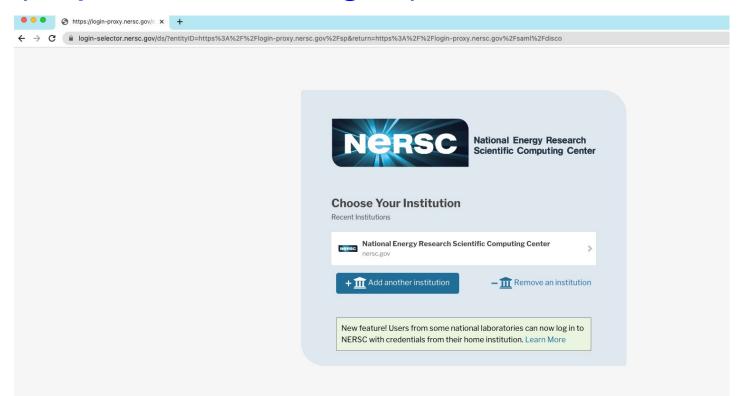








Iris (https://iris.nersc.gov) for Your Account

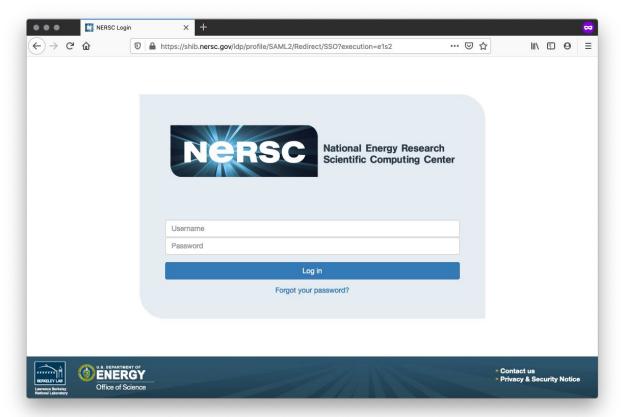








Iris (https://iris.nersc.gov) for Your Account









Multi-Factor Authentication (MFA)

Tip: you will use this a LOT

- Protects NERSC users from attacks like this →
- Log into NERSC resources with your NERSC password plus a one-time code that is provided by an app









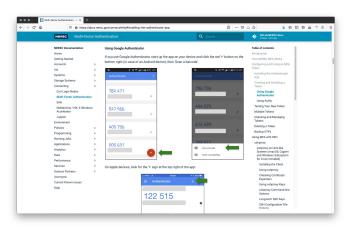
Setting Up MFA in Iris

 First install Google Authenticator on your smartphone (and/or Authy on your computer)

https://play.google.com/store/apps/details?id=com.google.android.apps.authenticator2&hl=enhttps://itunes.apple.com/us/app/google-authenticator/id388497605?mt=8

https://authy.com

Search "MFA" at https://docs.nersc.gov



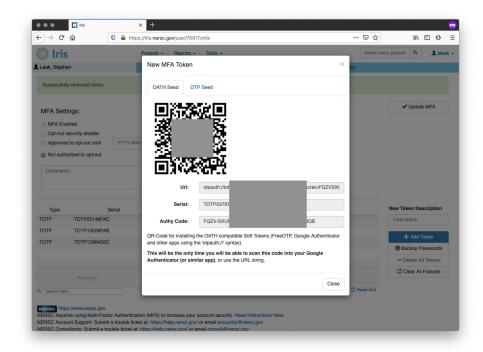






Setting Up MFA in Iris

- Click the "MFA" tab
- Click the "Add Token" button
- Scan the QR code with the Authenticator app (or, paste the Authy code into Authy)



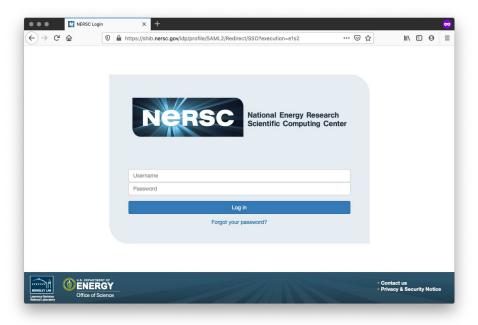






Logging in with MFA

After single-sign-on page you'll be asked for your one-time password (6 digits from app)



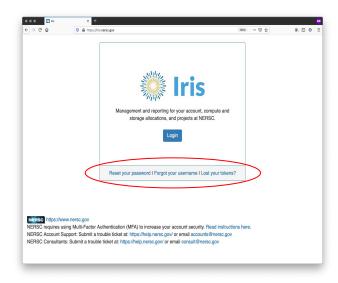






Troubleshooting Account Access

- I can't login to Iris
 - New account? It may not be approved yet (can take a few days)
 - Forgot password? Lost MFA tokens?
 Use the links on the Iris login page
- I can login to Iris, but not Cori or Perlmutter
 - Are you in a project? Check "Roles" tab



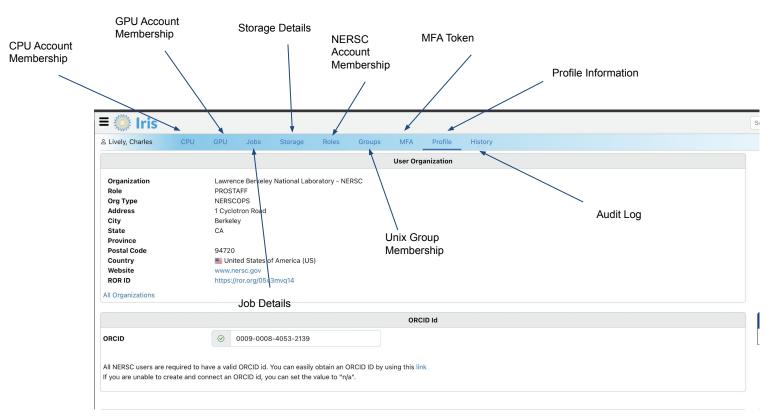








Navigating Iris - Menu Bar

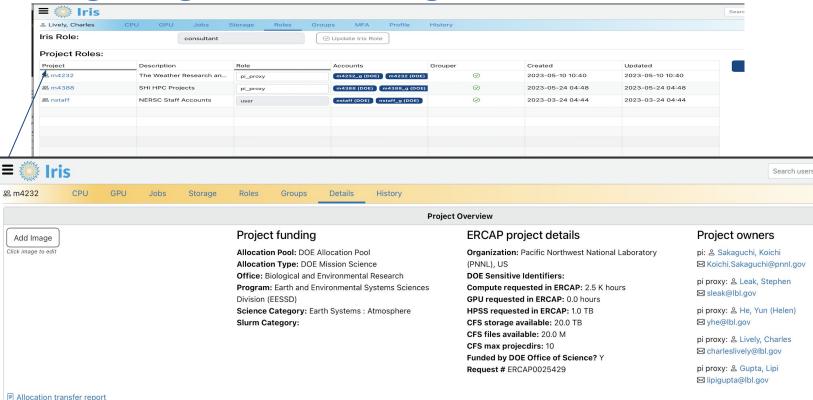








Navigating Iris - Finding Account Details









Navigating Iris - Changing User Shell

Ldap Tree	Home Directory	Login Shell	Username	GID	Group	Actions
alvarez	/global/homes/s/siddiq90	/bin/bash	siddiq90	92503	siddiq90	☑ Edit X Delete Q Search
ori	/global/homes/s/siddiq90	/bin/zsh	siddiq90	92503	siddiq90	☑ Edit X Delete Q Search
latatran	/global/homes/s/siddiq90	/bin/zsh	siddiq90	92503	siddiq90	☑ Edit X Delete Q Search
erty	/global/homes/s/siddiq90	/bin/zsh	siddiq90	92503	siddiq90	☑ Edit X Delete Q Search
pss	/home/s/siddiq90	/bin/bash	siddiq90	92503	siddiq90	☑ Edit X Delete Q Search
nuller	/global/homes/s/siddiq90	/bin/zsh	siddiq90	92503	siddiq90	☑ Edit X Delete Q Search
im-ldap	/home/siddiq90	/bin/bash	siddiq90	92503	siddiq90	☑ Edit Q Search
x	/global/homes/s/siddiq90	/bin/zsh	siddiq90	92503	siddiq90	☑ Edit X Delete Q Search
erlmutter	/global/homes/s/siddiq90	/bin/bash	siddiq90	92503	sidelq90	☑ Edit X Delete Q Search
erver	/home/siddiq90	/bin/bash	siddiq90	92503	siddiq90	☑ Edit X Delete Q Search
	Previous	Page 1	of 2	10 rows ~	Next	
Search table		⊕ .csv				♦ Option

Add a new Server Log	×	
	/bin/bash	
Server	/bin/csh	
	/bin/tcsh	h
Home Directory	/bin/ksh	
	/bin/sh	Ĭ,
Login Shell	✓ /bin/zsh	
Username	siddiq90	
GID	92503	
Group Name	siddiq90	

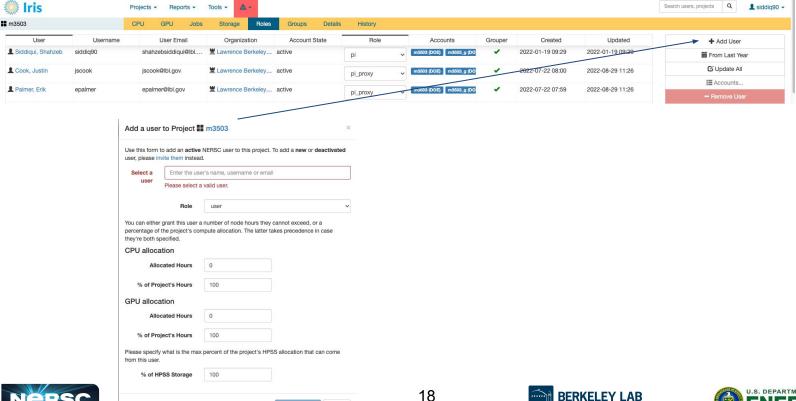






Navigating Iris - Adding User to Account

PI and PI Proxy only!









Cancel



Connecting with SSH





You will need a (text) terminal program!

- Mac: terminal (built-in) or "iTerm2" (https://www.iterm2.com/)
- Windows: PuTTY (https://mobaxterm.mobatek.net/) or XWin32 or Git BASH
- Linux: Your own favorite :)
- Chromebook: crosh (developer mode) or Crostini (Linux-in-a-container) or SSH App







Connecting to NERSC systems

Connect to NERSC Computational Systems

Please make sure you have configured Multi-Factor Authentication (MFA) prior to login.

To access Perlmutter via ssh you can do the following:

ssh <user>@perlmutter-p1.nersc.gov

or

ssh <user>@saul-p1.nersc.gov

Similarly, you can access Cori with

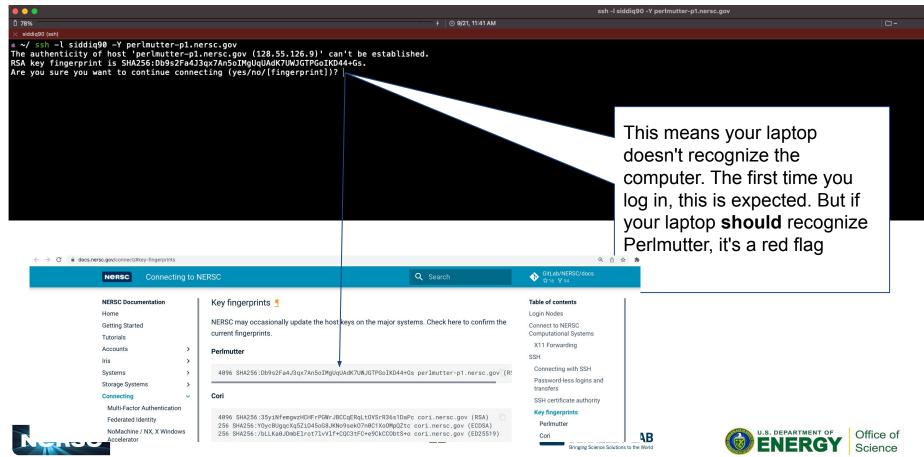
ssh <user>@cori.nersc.gov







Connecting with SSH



Connecting with SSH

When you ssh in, you'll see a prompt like:

Password + OTP:

Enter your (iris) password, then
the 6 digits from Authenticator, with no spaces etc between
Example: Pa\$\$w0rd!123456

Nothing will appear at prompt as you type! (this is normal) If you only get "Password: (no "+ OTP"), your account may not be ready yet





~/ ssh -l siddig90 -Y perlmutter-p1.nersc.gov

expectation of privacy.

stated in this warning.

Warning: Permanently added the RSA host key for IP address '128.55.126.12'

Lawrence Berkeley National Laboratory operates this computer system under contract to the U.S. Department of Energy. This computer system is the property of the United States Government and is for authorized use only. Users (authorized or unauthorized) have no explicit or implicit

as well as authorized officials of other agencies, both domestic and foreign. By using this system, the user consents to such interception, monitoring recording, copying, auditing, inspection, and disclosure at the discretion

Unauthorized or improper use of this system may result in administrative disciplinary action and civil and criminal penalties. By continuing to use this system you indicate your awareness of and consent to these terms and conditions of use. LOG OFF IMMEDIATELY if you do not agree to the conditions

Any or all uses of this system and all files on this system may be intercepted, monitored, recorded, copied, audited, inspected, and disclosed to authorized site, Department of Energy, and law enforcement personnel,

of authorized site or Department of Energy personnel.



SSH Options

Wait, what was that "-Y"?

```
1 78%

x siddiq90 (seh)

x ~/ ssh -l siddiq90 -Y perlmutter-p1.nersc.gov

The authenticity of host 'perlmutter-p1.nersc.gov (128.55.126.6)' can't be established.

RSA key fingerprint is SHA256:Db9s2Fa4J3qx7An5oIMgUqUAdK7UWJGTPGoIKD44+Gs.

Are you sure you want to continue connecting (yes/no/[fingerprint])?
```

```
"ssh -Y" (or "ssh -X") allow X (ie, GUI) programs to display on your local monitor.
```

- You need an X-server (http://x.cyqwin.com/ for Windows)
- Can be very slow alternatives coming up!

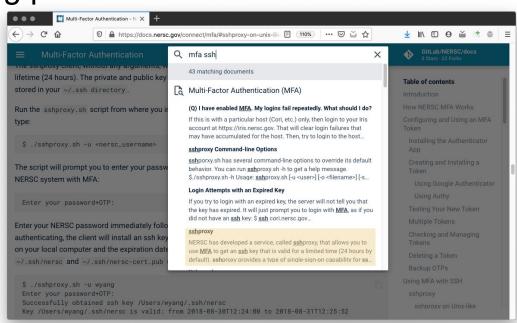






sshproxy

- Tired of repeatedly typing password + OTP?
 - sshproxy.sh creates a short-term (24 hours) certificate
 - Run sshproxy.sh
 once, then you can ssh
 to NERSC systems for
 the next 24 hours
 before being asked for
 password+OTP again



Search "MFA SSH" at https://docs.nersc.gov



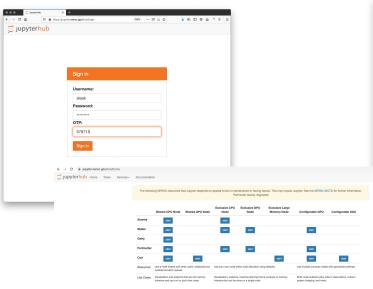


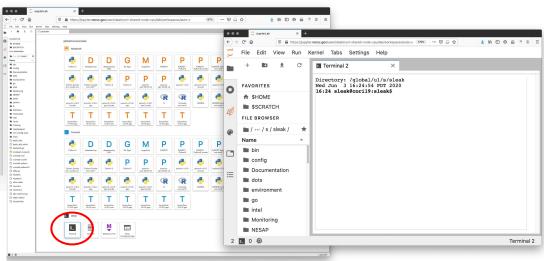


Jupyter

You can access NERSC systems from any web browser, via

https://jupyter.nersc.gov











Running GUI Apps

GUI apps eg Matlab, DDT (debugging), Nsight (performance) can be painfully slow over a network

SSH Options

Wait, what was that "-Y"?

"ssh -Y" (or "ssh -X")
allow X (ie, GUI) programs on Cori to display on your local
monitor.

- You need an X-server (<u>https://www.xquartz.org/</u> for Mac or <u>http://x.cygwin.com/</u> for Windows)
- Can be very slow alternatives coming up!



BERKELEY LAB



Why is this, and how can we fix it?









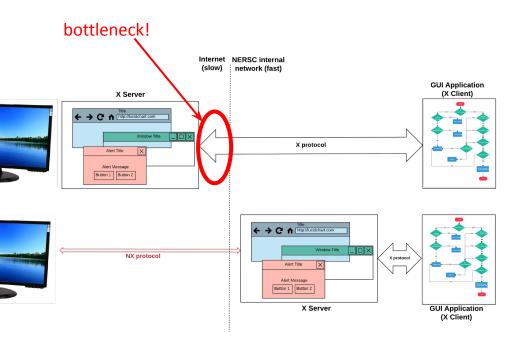
NoMachine: Accelerated X

X protocol makes a lot of traffic

OK over the (fast) network internal to NERSC

 Not OK over the (slow) internet

NoMachine runs **inside** NERSC, and sends less data over the (slow) internet



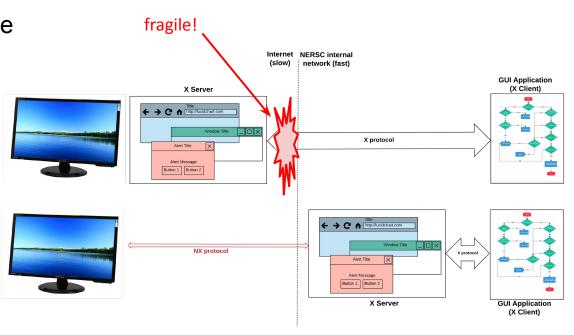






NoMachine: Accelerated X

NoMachine also removes the weakest link, so broken connections don't kill your application



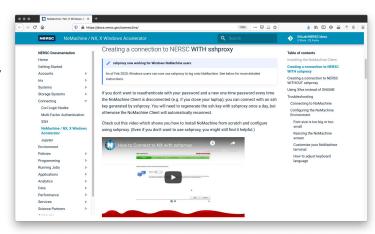






How to Set It Up

- https://docs.nersc.gov/connect/nx/ has detailed instructions
 - Download the client (https://www.nomachine.com/download-enterprise#NoMachine-Enterprise-Client)
 - (Make sure to get the **client**, not the server or workstation)
 - Setup a connection (can optionally use the key you generated with sshproxy.sh)







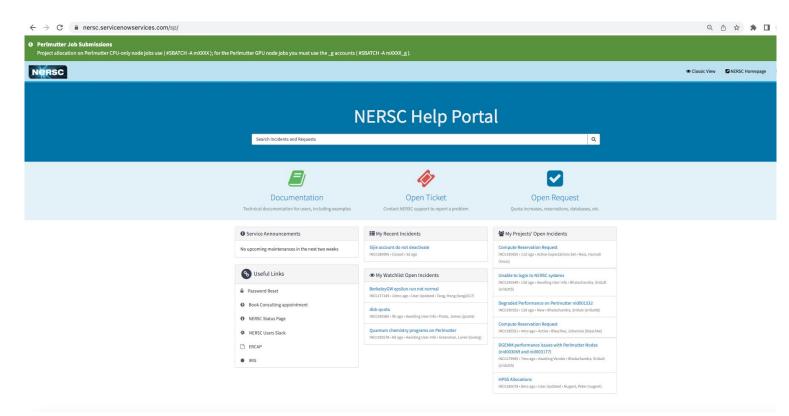


Getting Help! (Submitting a User Ticket)





NERSC Help Portal: https://help.nersc.gov/

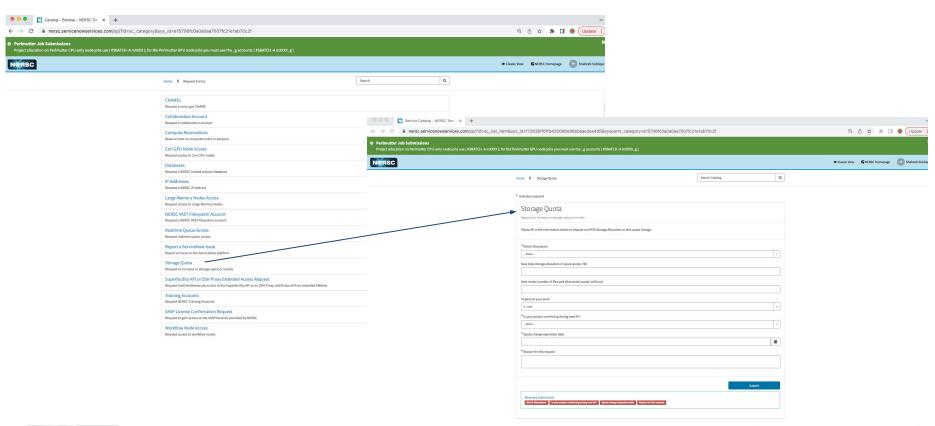








Request Forms









How to file a Good Ticket

Do Include:

- error messages, JobID, location of relevant files on system, output of module list
- Steps to reproduce

Don't Include:

 Screenshots! (This seems helpful but usually cannot be read easily, and can't copy/paste text from an image!)



Pasting a bare error message

Providing all the steps to reproduce

https://docs.nersc.gov/getting-started/#how-to-file-a-good-ticket







For Example!

Hard to troubleshoot

Better to troubleshoot

- → My code is slow
- → My job won't start
- → Perlmutter is broken



It's always helpful to include the actual error message, even if it's long!

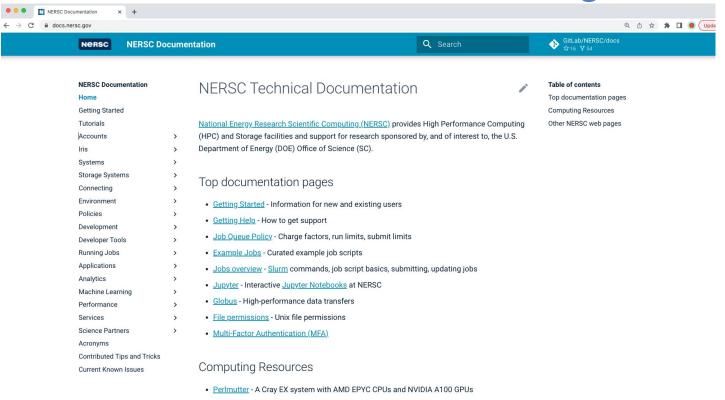
JobID 123456 was 3x slower than JobID 234566. The jobscript located at \$HOME/submit job.sh works on Cori but not on Perlmutter. This was the error message:... Running python \$SCRATCH/test cori.py crashes with this error message.









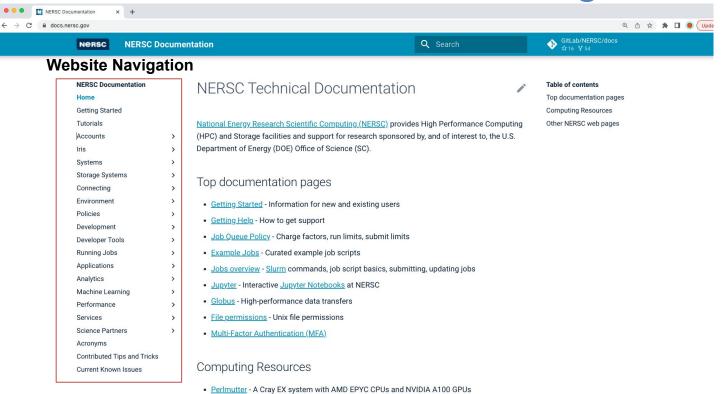








. Cori - A Cray XC40 system with Intel Haswell and Intel KNI CPUs

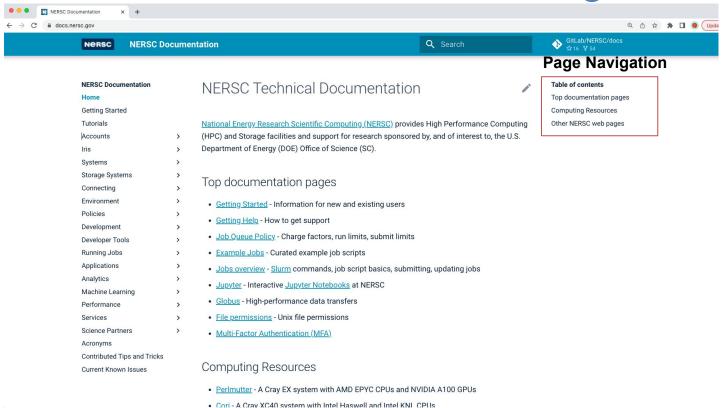








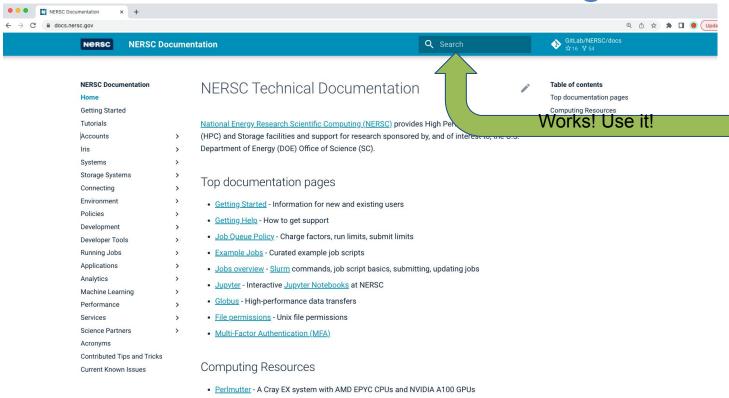
. Cori - A Cray XC40 system with Intel Haswell and Intel KNI CPUs











. Cori - A Cray XC40 system with Intel Haswell and Intel KNI CPUs







NERSC Documentation - System Overview

Nersc

NERSC Documentation

Q Search

→ GitLab/NERSC/docs



NERSC Systems

NERSC is one of the largest facilities in the world devoted to providing computational resources for scientific computing.

Perlmutter

<u>Perlmutter</u> is a HPE (Hewlett Packard Enterprise) Cray EX supercomputer, named in honor of Saul Perlmutter, an astrophysicist at Berkeley Lab who shared the 2011 Nobel Prize in Physics for his contributions to research showing that the expansion of the universe is accelerating.

Perlmutter, based on the HPE Cray Shasta platform, is a heterogeneous system comprising both CPU-only and GPU-accelerated nodes, with a performance of 3-4 times Cori when the installation completes.

We are in the process of Perlmutter Phase 2 integration (adding CPU only nodes and upgrading our system network to Slingshot 11). The final system will consist of 1536 GPU accelerated nodes with 1 AMD Milan processor and 4 NVIDIA A100 GPUs, and 3072 CPU-only nodes with 2 AMD Milan processors. The actual number of nodes available will be in flux during the integration and acceptance of the full system.

Cori (retired)

Cori, a Cray XC40 with a peak performance of about 30 petaflops, was retired on May 31, 2023. The system was named in honor of American biochemist <u>Gerty Cori</u>, the first American woman to win a Nobel Prize and the first woman to be awarded the prize in Physiology or Medicine.

Data transfer nodes

The <u>data transfer nodes</u> are NERSC servers dedicated to performing transfers between NERSC data storage resources such as HPSS and the NERSC Global File System (NGF) and storage

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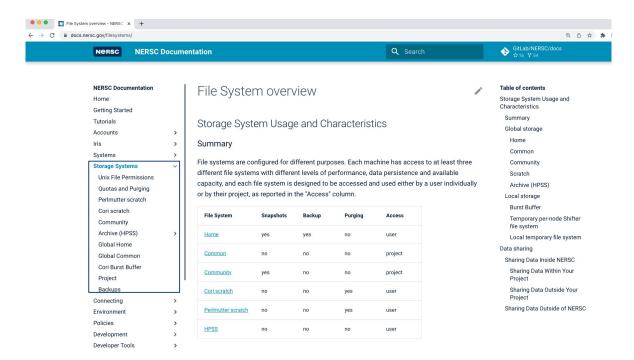
Perlmutter Cori (retired)

Data transfer nodes





NERSC Documentation - Storage Overview

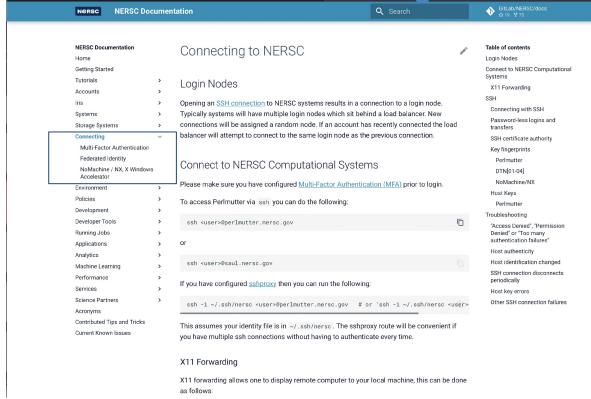








NERSC Documentation - Connecting to NERSC

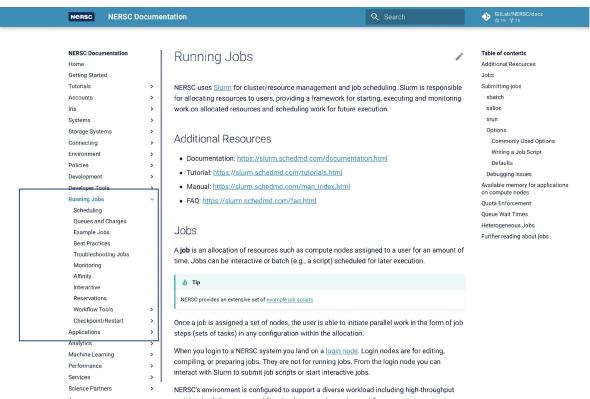








NERSC Documentation - Running Jobs









NERSC Documentation - Programming Models

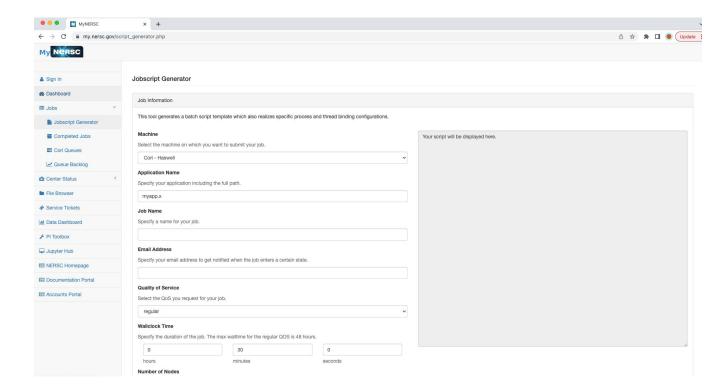
NERSC Documentation Q Search Nersc **NERSC Documentation** Programming Models Table of contents Home Parallel programming models at Getting Started Perlmutter, and beyond: Tutorials A wide variety of programming models are used on NERSC systems. The most common is MPI Performance and portability Accounts + OpenMP, but many others are supported. Why MPI + OpenMP? Iris Combining Programming Models Systems Distributed memory (inter-node) Parallel programming models at NERSC parallelism Storage Systems Shared memory (intra-node) Connecting Since the transition from vector to distributed memory (MPP) supercomputer architectures, the parallelism Environment majority of HPC applications deployed on NERSC resources have evolved to use MPI as their Policies sole means of expressing parallelism. As single processor core compute nodes on MPP Development architectures gave way to multicore processors, applying the same abstraction (processes Compilers passing messages) to each available core remained an attractive alternative - no code changes **Build Tools** were required, and vendors made an effort to design optimized fast-paths for on-node **Programming Models** communication. MPI > However, as on-node parallelism rapidly increases and competition for shared resources per OpenMP processing element (memory per core, bandwidth per core, etc.) does as well, now is a good OpenACC time to assess whether applications can benefit from a different abstraction for expressing on-CUDA node parallelism. Examples of desirable functionality potentially available through the latter HPC include more efficient utilization of resources (e.g. through threading) or the ability to exploit UPC++ urique architectural features (e.g. vectorization). Coarrays SYCL Kokkos Perlmutter, and beyond: Performance and portability HPX Raia Perlmutter has a mixture of CPU-only nodes and CPU + GPU nodes. Each CPU + GPU nodes C++ parallel algorithms has 4 GPUs per CPU node. benchmark NERSC has made an effort to provide guidance on parallel programming approaches. Chief Languages among these is the combination of MPI for inter-node parallelism and OpenMP for intra-node Libraries parallelism (or potentially MPI per NUMA domain with OpenMP within each). Containers Developer Tools







Jobscript Generator



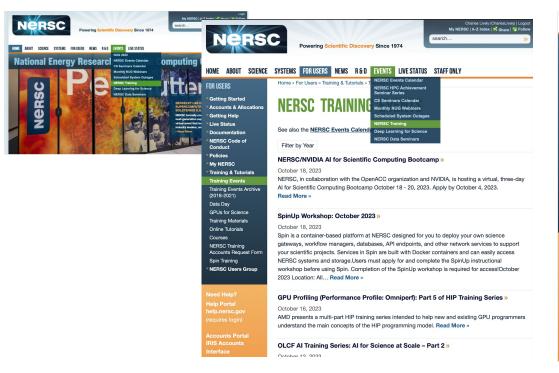








Navigating www.nersc.gov (NERSC Training)



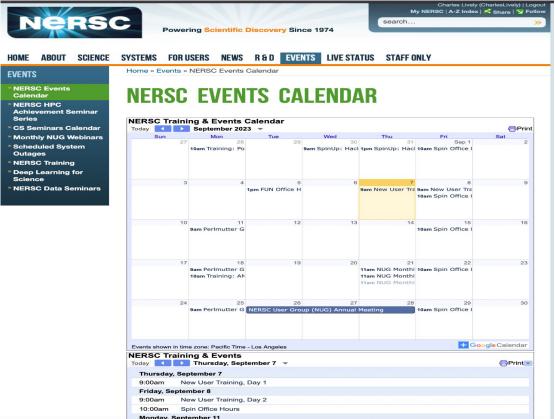








Navigating www.nersc.gov (NERSC Events)

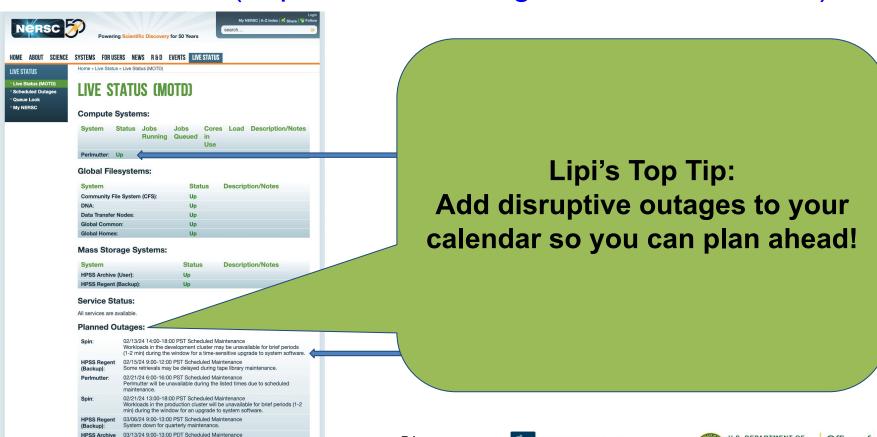








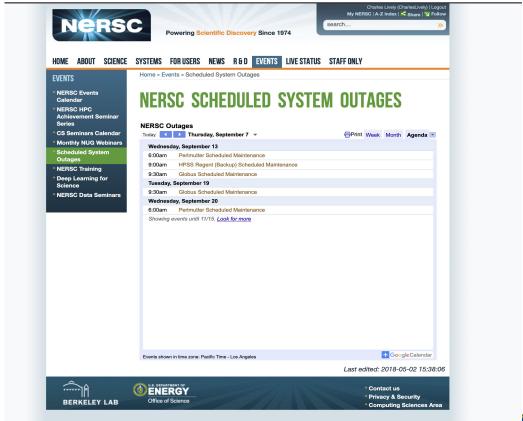
Live Status: (https://www.nersc.gov/live-status/motd/)





System down for quarterly maintenance.

Navigating www.nersc.gov (Scheduled System Outages)







Navigating www.nersc.gov (NERSC User Slack)

