Navigating and Connecting to NERSC

New User Training
February 15, 2024

Lipi Gupta, PhD
Science Engagement Engineer
User Engagement Group
What NOT to do!

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

some random cable from laptop to server rack?
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](https://iris.nersc.gov))
- Connecting to Perlmutter
  - Connecting with SSH
  - [https://jupyter.nersc.gov](https://jupyter.nersc.gov) notebooks and terminals in your browser
  - NoMachine ([https://docs.nersc.gov/connect/nx/](https://docs.nersc.gov/connect/nx/)) for GUI apps
- Submitting a User Ticket ([https://help.nersc.gov](https://help.nersc.gov))
- Navigating NERSC Documentation
- Navigating NERSC Home Page
Navigating Iris
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](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://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
  o New account? It may not be approved yet (can take a few days)
  o Forgot password? Lost MFA tokens?
    Use the links on the Iris login page

• I can login to Iris, but not Cori or Perlmutter
  o Are you in a project? Check "Roles" tab
Navigating Iris - Menu Bar

- CPU Account Membership
- GPU Account Membership
- Storage Details
- NERSC Account Membership
- MFA Token
- Profile Information

User Organization

Audit Log

Unix Group Membership

Job Details

ORCID

All NERSC users are required to have a valid ORCID id. You can easily obtain an ORCID ID by using this link. If you are unable to create and connect an ORCID id, you can set the value to "n/a".

ORCID

0009-0008-4053-2199

15
Navigating Iris - Finding Account Details

**Project Overview**

**Project funding**
- **Allocation Pool**: DOE Allocation Pool
- **Allocation Type**: DOE Mission Science
- **Office**: Biological and Environmental Research
- **Program**: Earth and Environmental Systems Sciences
- **Science Category**: Earth Systems: Atmosphere
- **Slurm Category**:

**ERCAP project details**
- **Organization**: Pacific Northwest National Laboratory (PNNL), US
- **DOE Sensitive Identifiers**:
  - Compute requested in ERCAP: 2.5 K hours
  - GPU requested in ERCAP: 0.0 hours
  - HPSS requested in ERCAP: 1.0 TB
  - CFS storage available: 200 TB
  - CFS files available: 20.0 M
  - CFS max projectdirs: 10
- **Funded by DOE Office of Science?** Y
- **Request #**: ERCAP0025429

**Project owners**
- pi: & Sakaguchi, Koichi  
  - Koichi.Sakaguchi@pnnl.gov
- pi proxy: & Leak, Stephen  
  - sleak@lbl.gov
- pi proxy: & He, Yun (Helen)  
  - yhe@lbl.gov
- pi proxy: & Lively, Charles  
  - charleslively@lbl.gov
- pi proxy: & Gupta, Lipi  
  - lipigupta@lbl.gov
Navigating Iris - Changing User Shell
Navigating Iris - Adding User to Account

PI and PI Proxy only!

<table>
<thead>
<tr>
<th>User</th>
<th>Username</th>
<th>User Email</th>
<th>Organization</th>
<th>Account State</th>
<th>Role</th>
<th>Accounts</th>
<th>Groupers</th>
<th>Created</th>
<th>Updated</th>
</tr>
</thead>
<tbody>
<tr>
<td>Siddiqui, Shafeeq</td>
<td>siddiq90</td>
<td><a href="mailto:siddiq@lbl.gov">siddiq@lbl.gov</a></td>
<td>Lawrence Berkeley...</td>
<td>active</td>
<td>pi</td>
<td>user</td>
<td>user</td>
<td>2022-01-19 09:29</td>
<td>2022-01-19 09:29</td>
</tr>
<tr>
<td>Cook, Justin</td>
<td>jcook</td>
<td><a href="mailto:jcook@lbl.gov">jcook@lbl.gov</a></td>
<td>Lawrence Berkeley...</td>
<td>active</td>
<td>pi_proxy</td>
<td>user</td>
<td>user</td>
<td>2022-07-22 08:00</td>
<td>2022-08-29 11:26</td>
</tr>
<tr>
<td>Palmer, Erik</td>
<td>epalmer</td>
<td><a href="mailto:epalmer@lbl.gov">epalmer@lbl.gov</a></td>
<td>Lawrence Berkeley...</td>
<td>active</td>
<td>pi_proxy</td>
<td>user</td>
<td>user</td>
<td>2022-07-22 07:39</td>
<td>2022-08-29 11:28</td>
</tr>
</tbody>
</table>

Add a user to Project m3503

Use this form to add an active NERSC user to this project. To add a new or deactivated user, please invite them instead.

Select a user
Enter the user’s name, username or email
Please select a valid user:

Role

CPU allocation
- Allocated Hours
- % of Project's Hours

GPU allocation
- Allocated Hours
- % of Project's Hours

Please specify what is the max percent of the project's HPSS allocation that can come from this user:
- % of HPSS Storage

Save Changes  Cancel
Connecting to NERSC Systems
Connecting with SSH

You will need a *text* terminal program!

- Mac: terminal (built-in) or "iTerm2" ([https://www.iterm2.com/](https://www.iterm2.com/))
- 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

This means your laptop doesn't recognize the computer. The first time you log in, this is expected. But if your laptop **should** recognize Perlmutter, it's a red flag.
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: \texttt{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 Options

Wait, what was that "-Y"?

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

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

• Tired of repeatedly typing password + OTP?
  o **sshproxy.sh** creates a short-term (24 hours) certificate
  o 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](https://docs.nersc.gov)
You can access NERSC systems from any web browser, via [https://jupyter.nersc.gov](https://jupyter.nersc.gov)
Running GUI Apps

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

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/](https://docs.nersc.gov/connect/nx/) has detailed instructions
  - Download the client ([https://www.nomachine.com/download-enterprise#NoMachine-Enterprise-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/](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!)

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

Hard to troubleshoot

→ My code is slow
→ My job won’t start
→ Perlmutter is broken

Better to troubleshoot

→ 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.

It’s always helpful to include the actual error message, even if it’s long!
NERSC Technical Documentation

National Energy Research Scientific Computing (NERSC) provides High Performance Computing (HPC) and Storage facilities and support for research sponsored by, and of interest to, the U.S. Department of Energy (DOE) Office of Science (SC).

Top documentation pages

- Getting Started - Information for new and existing users
- Getting Help - How to get support
- Job Queue Policy - Charge factors, run limits, submit limits
- Example Jobs - Curated example job scripts
- Jobs overview - Slurm commands, job script basics, submitting, updating jobs
- Juno - Interactive Juno Notebooks at NERSC
- Globus - High-performance data transfers
- File permissions - Unix file permissions
- Multi-Factor Authentication (MFA)

Computing Resources

- Perlmutter - A Cray EX system with AMD EPYC CPUs and NVIDIA A100 GPUs
- Cori - A Cray XD system with Intel Haswell and Intel X86 CPUs
NERSC Documentation - Main Page

Website Navigation

NERSC Technical Documentation

National Energy Research Scientific Computing (NERSC) provides High Performance Computing (HPC) and Storage facilities and support for research sponsored by, and of interest to, the U.S. Department of Energy (DOE) Office of Science (SC).

Top documentation pages

- **Getting Started** - Information for new and existing users
- **Getting Help** - How to get support
- **Job Queue Policy** - Charge factors, run limits, submit limits
- **Example Jobs** - Curated example job scripts
- **Jobs overview** - Slurm commands, job script basics, submitting, updating jobs
- **Jupyter** - Interactive Jupyter Notebooks at NERSC
- **Globus** - High-performance data transfers
- **File permissions** - Unix file permissions
- **Multi-Factor Authentication (MFA)**

Computing Resources

- **Perlmutter** - A Cray EX system with AMD EPYC CPUs and NVIDIA A100 GPUs
- **Cori** - A Cray XC40 system with Intel Haswell and Intel XEON CPUs
NERSC Technical Documentation

National Energy Research Scientific Computing (NERSC) provides High Performance Computing (HPC) and Storage facilities and support for research sponsored by, and of interest to, the U.S. Department of Energy (DOE) Office of Science (SC).

Top documentation pages

- Getting Started - Information for new and existing users
- Getting Help - How to get support
- Job Queue Policy - Charge factors, run limits, submit limits
- Example Jobs - Curated example job scripts
- Jobs overview - Slurm commands, job script basics, submitting, updating jobs
- Jupyter - Interactive Jupyter Notebooks at NERSC
- Globus - High-performance data transfers
- File permissions - Unix file permissions
- Multi-Factor Authentication (MFA)

Computing Resources

- Perlmutter - A Cray EX system with AMD EPYC CPUs and NVIDIA A100 GPUs
- Cori - A Cray XC40 system with Intel Haswell and Intel XKB CPUs
NERSC Technical Documentation

National Energy Research Scientific Computing (NERSC) provides High Performance Computing (HPC) and Storage facilities and support for research sponsored by, and of interest to, the U.S. Department of Energy (DOE) Office of Science (SC).

Top documentation pages

- **Getting Started** - Information for new and existing users
- **Getting Help** - How to get support
- **Job Queue Policy** - Charge factors, run limits, submit limits
- **Example Jobs** - Curated example job scripts
- **Jobs overview** - Slurm commands, job script basics, submitting, updating jobs
- **Jupyter** - Interactive Jupyter Notebooks at NERSC
- **Globus** - High-performance data transfers
- **File permissions** - Unix file permissions
- **Multi-Factor Authentication (MFA)**

Computing Resources

- **Perlmutter** - A Cray EX system with AMD EPYC CPUs and NVIDIA A100 GPUs
- **Cori** - A Cray XC40 system with Intel Haswell and Intel Xeon Phi

Works! Use it!
NERSC Systems

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

Perlmutter

Perlmutter 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 Gerty Cori, 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 data transfer nodes are NERSC servers dedicated to performing transfers between NERSC data storage resources such as NGGF and the NERSC Global File System (NGFS), and storage
File System overview

Storage System Usage and Characteristics

Summary

File systems are configured for different purposes. Each machine has access to at least three different file systems with different levels of performance, data persistence and available capacity, and each file system is designed to be accessed and used either by a user individually or by their project, as reported in the 'Access' column.

<table>
<thead>
<tr>
<th>File System</th>
<th>Snapshots</th>
<th>Backup</th>
<th>Purging</th>
<th>Access</th>
</tr>
</thead>
<tbody>
<tr>
<td>Home</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
<td>user</td>
</tr>
<tr>
<td>Community</td>
<td>no</td>
<td>no</td>
<td>no</td>
<td>project</td>
</tr>
<tr>
<td>Perlmutter scratch</td>
<td>yes</td>
<td>no</td>
<td>yes</td>
<td>user</td>
</tr>
<tr>
<td>HPSS</td>
<td>no</td>
<td>no</td>
<td>no</td>
<td>user</td>
</tr>
</tbody>
</table>
Connecting to NERSC

Login Nodes

Opening an SSH connection to NERSC systems results in a connection to a login node. Typically systems will have multiple login nodes which sit behind a load balancer. New connections will be assigned a random node. If an account has recently connected the load balancer will attempt to connect to the same login node as the previous connection.

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.nersc.gov
```

or

```
ssh <user>@eaudl.nersc.gov
```

If you have configured `submerge` then you can run the following:

```
ssh -i ~/.ssh/nersc <user>@perlmutter.nersc.gov  # or `ssh -i ~/.ssh/nersc <user>
```

This assumes your identity file is in `~/.ssh/nersc`. The sshproxy route will be convenient if you have multiple ssh connections without having to authenticate every time.

X11 Forwarding

X11 forwarding allows one to display remote computer to your local machine, this can be done as follows:
Running Jobs

NERSC uses **Slurm** for cluster/resource management and job scheduling. Slurm is responsible for allocating resources to users, providing a framework for starting, executing and monitoring work on allocated resources and scheduling work for future execution.

Additional Resources

- Documentation: [https://slurm.schedmd.com/documentation.html](https://slurm.schedmd.com/documentation.html)
- Tutorial: [https://slurm.schedmd.com/tutorials.html](https://slurm.schedmd.com/tutorials.html)
- Manual: [https://slurm.schedmd.com/man_index.html](https://slurm.schedmd.com/man_index.html)
- FAQ: [https://slurm.schedmd.com/faq.html](https://slurm.schedmd.com/faq.html)

Jobs

A **job** is an allocation of resources such as compute nodes assigned to a user for an amount of time. Jobs can be interactive or batch (e.g., a script) scheduled for later execution.

**Tip**

NERSC provides an extensive set of **example job scripts**

Once a job is assigned a set of nodes, the user is able to initiate parallel work in the form of job steps (sets of tasks) in any configuration within the allocation.

When you login to a NERSC system you land on a **login node**. Login nodes are for editing, compiling, or preparing jobs. They are not for running jobs. From the login node you can interact with Slurm to submit job scripts or start interactive jobs.

NERSC's environment is configured to support a diverse workload including high-throughput computation.
Programming Models

A wide variety of programming models are used on NERSC systems. The most common is MPI + OpenMP, but many others are supported.

Parallel programming models at NERSC

Since the transition from vector to distributed memory (MPP) supercomputer architectures, the majority of HPC applications deployed on NERSC resources have evolved to use MPI as their sole means of expressing parallelism. As single processor core compute nodes on MPP architectures gave way to multicore processors, applying the same abstraction (processes passing messages) to each available core remained an attractive alternative - no code changes were required, and vendors made an effort to design optimized fast-paths for on-node communication.

However, as on-node parallelism rapidly increases and competition for shared resources per processing element (memory per core, bandwidth per core, etc.) does as well, now is a good time to assess whether applications can benefit from a different abstraction for expressing on-node parallelism. Examples of desirable functionality potentially available through the latter include more efficient utilization of resources (e.g. through threading) or the ability to exploit unique architectural features (e.g. vectorization).

Perlmutter, and beyond: Performance and portability

Perlmutter has a mixture of CPU-only nodes and CPU + GPU nodes. Each CPU + GPU node has 4 GPUs per CPU node.

NERSC has made an effort to provide guidance on parallel programming approaches. Chief among these is the combination of MPI for inter-node parallelism and OpenMP for intra-node parallelism (or potentially MPI per NUMA domain with OpenMP within each).
Navigating NERSC Home Page
Navigating www.nersc.gov (NERSC Events)
Live Status: [https://www.nersc.gov/live-status/motd/](https://www.nersc.gov/live-status/motd/)

Lipi’s Top Tip:
Add disruptive outages to your calendar so you can plan ahead!
Navigating www.nersc.gov (Scheduled System Outages)

NERSC SCHEDULED SYSTEM OUTAGES

NERSC Outages

Wednesday, September 7

6:00am  Perlmutter Scheduled Maintenance
9:00am  HPSB Regent (Backup) Scheduled Maintenance
9:30am  Globus Scheduled Maintenance

Tuesday, September 19

9:30am  Globus Scheduled Maintenance

Wednesday, September 20

6:00am  Perlmutter Scheduled Maintenance

Events shown in time zone: Pacific Time - Los Angeles

Last edited: 2018-05-02 15:38:06

[Image of NERSC website with scheduled system outages]

NERSC
Powering Scientific Discovery Since 1974

HOME  ABOUT  SCIENCE  SYSTEMS  FOR USERS  NEWS  R&D  EVENTS  LIVE STATUS  STAFF ONLY

NERSC Events Calendar
NERSC HPC Achievement Seminar Series
CS-Seminar Calendar
Monthly NUG Webinars

Events
NERSC Events Calendar
NERSC HPC Achievement Seminar Series
CS Seminars Calendar
Monthly NUG Webinars
Scheduled System Outages
NERSC Training
Deep Learning for Science
NERSC Data Seminars

Events
NERSC SCHEDULED SYSTEM OUTAGES
NERSC Outages
Wednesday, September 7
6:00am  Perlmutter Scheduled Maintenance
9:00am  HPSB Regent (Backup) Scheduled Maintenance
9:30am  Globus Scheduled Maintenance

Tuesday, September 19
9:30am  Globus Scheduled Maintenance

Wednesday, September 20
6:00am  Perlmutter Scheduled Maintenance

Events shown in time zone: Pacific Time - Los Angeles

Last edited: 2018-05-02 15:38:06

[Image of NERSC website with scheduled system outages]
Navigating www.nersc.gov (NERSC User Slack)
Thank You and Welcome to NERSC!