

# Getting Started on Perlmutter@NERSC NUG Community Call



NERSC Welcome and Overview  
May 22, 2024

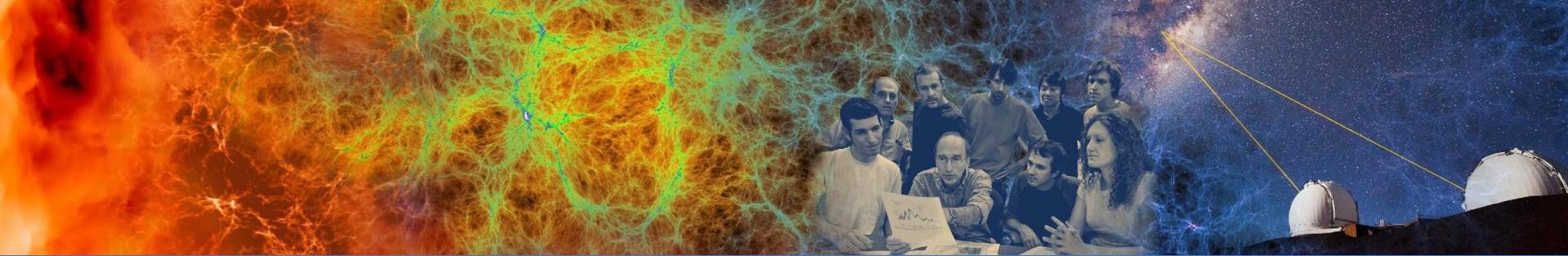
Charles Lively III, PhD & Lipi Gupta, PhD  
Science Engagement Engineers  
User Engagement Group (UEG)

# Agenda

- Welcome & Introduction to NERSC
- Hardware
- Software
- Interacting with NERSC
- Setting Up Your Account!

# Learning Outcomes

- Be able to describe the role of NERSC in the scientific research and computing landscape.
- Understand and identify computational resources at NERSC, both hardware and software.
- Be able to demonstrate how to submit a consulting ticket
- Set up your Multi-Factor Authentication and Password



# Introduction to NERSC

# About NERSC

- National Energy Research Scientific Computing Center
  - Established 1974, first unclassified supercomputer center
    - Original mission: to enable computational science as complement to magnetically controlled plasma experiment
  - 2024: NERSC 50th anniversary!
- Today's mission: ***Accelerate scientific discovery at the DOE Office of Science through High-Performance Computing and Extreme Data Analysis***
- NERSC is a national user facility
- NERSC is part of Berkeley Lab



# NERSC: Mission HPC for DOE Office of Science Research

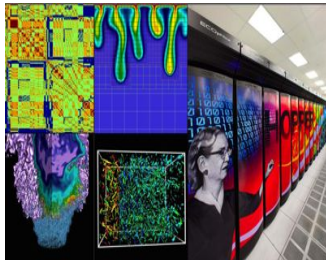


Office of  
Science

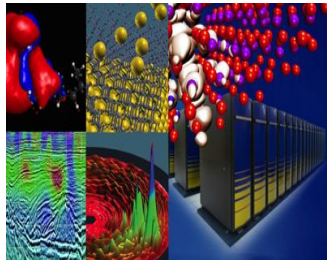
Largest funder of physical  
science research in U.S.



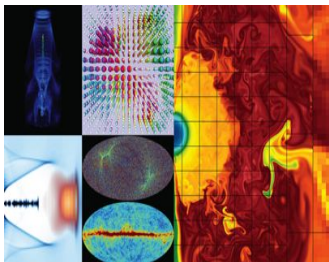
Bio Energy, Environment



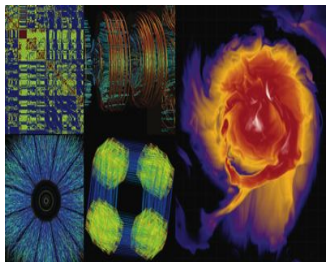
Computing



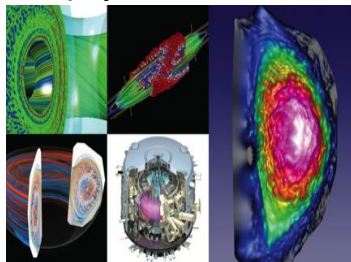
Materials, Chemistry,  
Geophysics



Particle Physics,  
Astrophysics



Nuclear Physics



Fusion Energy,  
Plasma Physics

Scientists all around the  
globe do their science on  
our machines!

We offer thousands of  
computational hours for a  
variety of scientific research.



# NERSC by the Numbers

## NERSC USERS ACROSS US AND WORLD

**50**  
States,  
Washington D.C.  
& Puerto Rico

**53**  
Countries

**~10,000** Annual Users from **~800** Institutions + National Labs



**32%**  
Graduate  
Students



**19%**  
Postdoctoral  
Fellows



**15%**  
Staff  
Scientists



**13%**  
University  
Faculty



**8%**  
Undergraduate  
Students



**5%**  
Professional  
Staff



**60%**  
Universities



**29%**  
DOE Labs



**5%**  
Other  
Government Labs



**4%**  
Industry

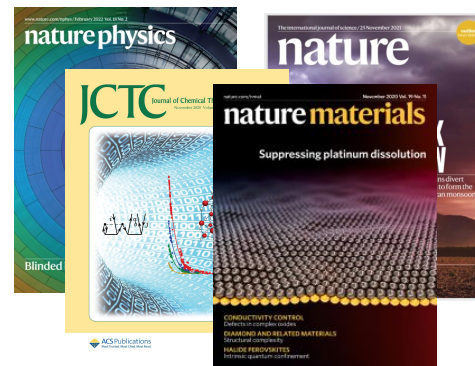


**1%**  
Small  
Businesses



**<1%**  
Private Labs

2,500 Referred Publications per Year



# Science Engagement @ NERSC



Lipi Gupta, PhD - Science Engagement Engineer



**Background:** PhD in Physics, University of Chicago

**Research Interests:** applying Machine Learning techniques to improve particle accelerator operation and control

**Eating Preferences/Fav Foods:** any noodle based dish!

**Favorite Sci-Fi Movie:** The Martian (2015 - Matt Damon and Jessica Chastain)

Charles Lively III, PhD



**Background:** PhD in Computer Engineering, Texas A&M University

**Research Interests:** Energy-Aware Computing, Performance Modeling and Optimization, Applications of Game Theory

**Eating Preferences/Fav Foods:** Vegan but seafood on rare occasions

**Favorite Sci-Fi Movie:** Contact (1997 - Jodie Foster and Matthew McConaughey)



# Nobel-Prize Winning Users



*for the development of multiscale models for complex chemical systems*

2013 Chemistry

Martin  
Karplus



*for the discovery of the accelerating expansion of the Universe through observations of distant supernovae*

2011 Physics

Saul Perlmutter



*for the discovery of the blackbody form and anisotropy of the cosmic microwave background radiation*

2006 Physics

George Smoot



*for their efforts to build up and disseminate greater knowledge about man-made climate change*

2007 Peace

Warren Washington



*for developing cryo-electron microscopy for the high-resolution structure determination of biomolecules in solution*

2017 Chemistry

Joachim Frank

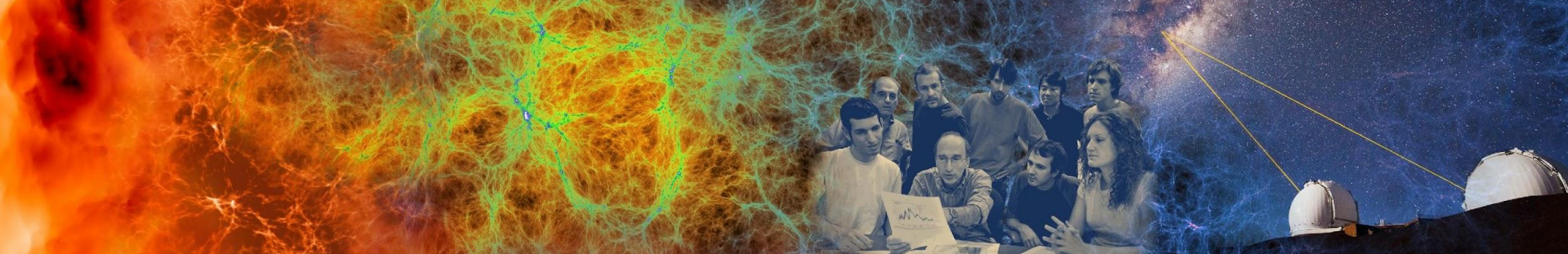


*for the discovery of neutrino oscillations, which shows that neutrinos have mass*

2015 Physics

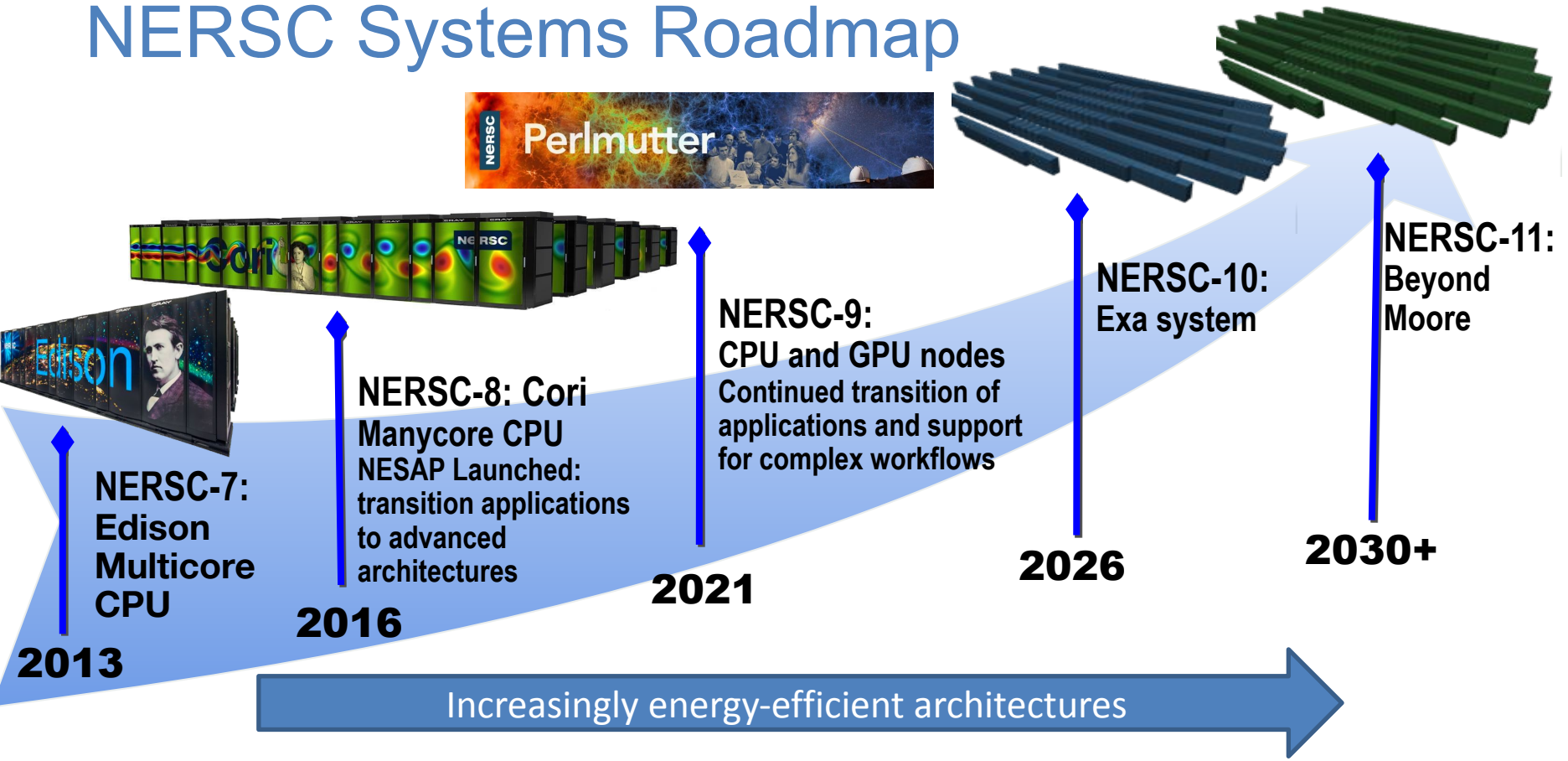
SNO Collaboration





# Hardware

# NERSC Systems Roadmap



# NERSC PERLMUTTER

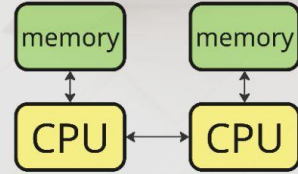
- Shared 2011 Nobel Prize in Physics for discovery of the accelerating expansion of the universe.
- Supernova Cosmology Project, lead by Perlmutter, was a pioneer in using NERSC supercomputers combine large scale simulations with experimental data analysis
- Login “saul.nerisc.gov”



**Login to Perlmutter**

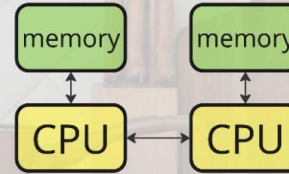
### Login Node

Only for logging in and  
basic tasks like submitting  
jobs to the job scheduler  
(not for running  
computation!)



### CPU-only Nodes

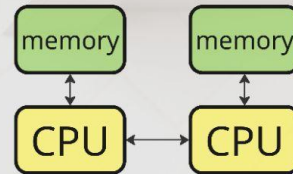
3072 Nodes on Perlmutter  
Architecture: 2 AMD EPYC 7763 CPUs per node  
Memory per node: 512 GB



## Login to Perlmutter

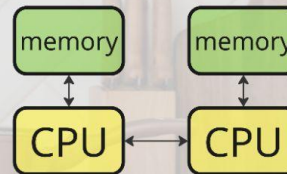
### Login Node

Only for logging in and basic tasks like submitting jobs to the job scheduler (not for running computation!)



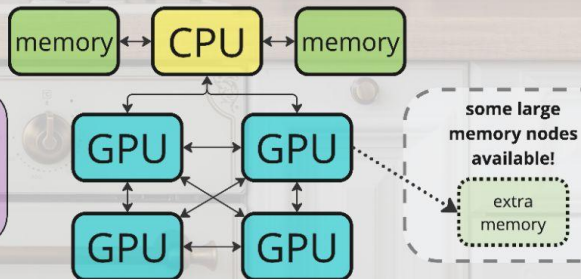
### CPU-only Nodes

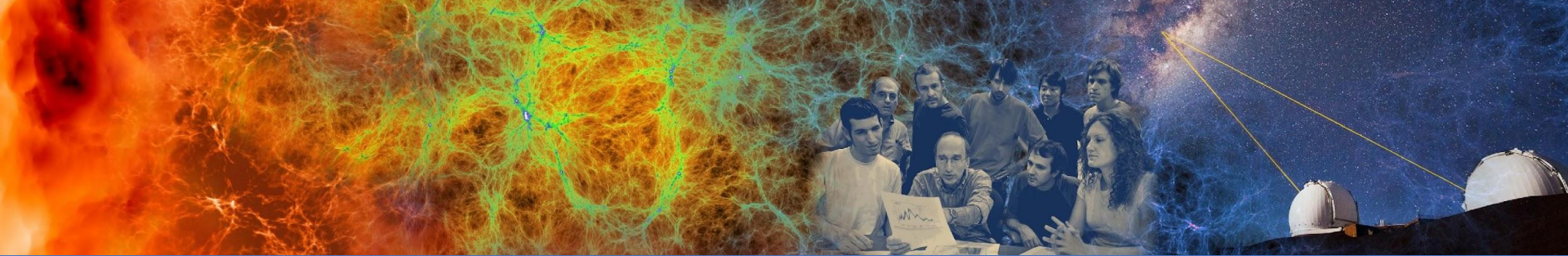
3072 Nodes on Perlmutter  
Architecture: 2 AMD EPYC 7763 CPUs per node  
Memory per node: 512 GB



### GPU Nodes

1794 Nodes (includes 256 large-memory GPU Nodes)  
Architecture: 1 AMD EPYC 7763 CPUs and 4 NVIDIA A100 GPUs  
Memory per Node: 256 GB (40 GB / 80 GB per large-memory GPU)





# Software

# Software

## NERSC-provided software

- AMBER
- Abinit
- BerkeleyGW
- CP2K
- E4S
- GAMESS
- Gromacs
- LAMMPS
- Mathematica
- MATLAB
- MOLPRO
- NAMD
- NCL
- NWChem
- ORCA
- SIESTA
- ParaView
- Q-Chem
- Quantum ESPRESSO
- VASP
- Wannier90
- WRF

<https://docs.nersc.gov/applications/>

## Bring Your Own!

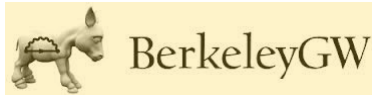
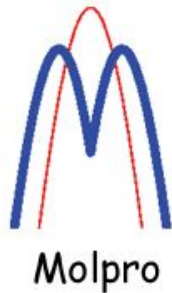
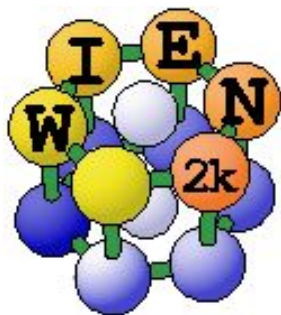
- Compile your own code using **our compiler wrappers**
- Easily use Python packages via conda environments
- Submit a request to have NERSC staff install software for you!



# Software

- Cray supercomputers OS is a version of Linux
- Compilers are provided on machines
- NERSC strategically provides software to users
- Libraries: many libraries are provided by vendor, still others provided by NERSC
- Applications: NERSC compiles and supports many software packages for our users
- Extreme-scale Scientific Software Stack (E4S) at NERSC is a curated software stack contains hundreds of packages delivered via the SPACK package manager

# Chemistry & Materials Science Applications



*abinit.*

- *More than 13.5 million lines of source code Compiled, Optimized, and Tested*



**NAMD**  
Scalable Molecular Dynamics

**VASP**  
b-initio  
package  
simulation  
lenna

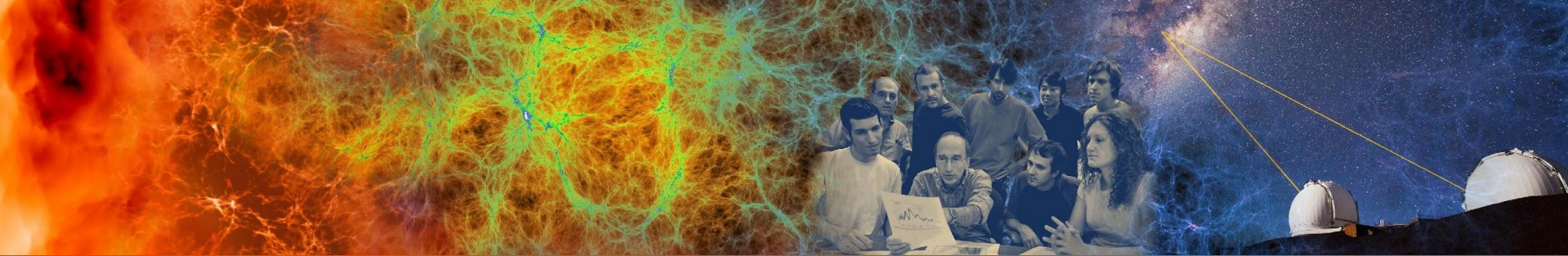
**GAMMESS**

**CPMD**

**LAMMPS**

**WANNIER90**





# Interacting with NERSC



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U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

# Interacting with NERSC

- NERSC User Engagement Group
  - User Engagement
  - User Training and Documentation
- NERSC Support
  - User Tickets
  - User Appointments
- NERSC Operations

# User Engagement Group - Our People



Lisa Claus



Kevin Gott



Lipi Gupta



Rebecca Hartman-Baker  
**UEG Group Lead**

## Alumni:

Tiffany Connors  
Zhengji Zhao  
Steve Leak  
Erik Palmer  
Justin Cook  
Shahzeb Siddiqui



Helen He

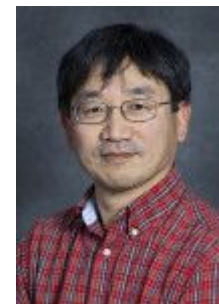


Charles Lively



Kelly Rowland

Kadidia Konate



Woo-Sun Yang

# NERSC User Group (NUG)

- Community of NERSC users
- Source of advice and feedback for NERSC (we listen!)
- Regular teleconferences hosted by NERSC
- Join the NUG Slack:  
<https://www.nersc.gov/users/NUG/nersc-users-slack/>
- Join us NUG Annual Meeting (Oct 22-24, 2024) for our 50th anniversary!



# NERSC User Training

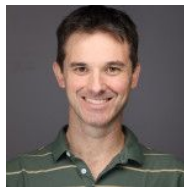
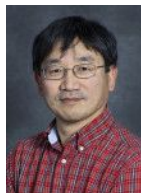
- NERSC provides a robust training program for users of all skill levels, interests, and personas
  - All trainings are recorded, professionally captioned, & posted to [NERSC YouTube channel](#)
  - Slides posted to training event webpage
- For more information on upcoming and past events, see <https://www.nersc.gov/users/training/events/>
- Collection of [Categorized Training Materials](#)
- [Training Events Archive](#)

# Interacting with NERSC

- NERSC User Engagement Group
  - User Engagement
  - User Training
- NERSC Support
  - User Tickets
  - User Appointments
- NERSC Operations



# Consulting & Account Support Team



# NERSC Consulting: Tips & Tricks

- Help us help you!
- Provide specifics:
  - What is the problem?
  - What machine? Which node? Which file path?
  - When did it happen?
  - What modules were loaded?
  - How did you try to fix or work around it?
  - How can I reproduce the problem?
- Tips for filing a good ticket:  
<https://docs.nersc.gov/getting-started/#how-to-file-a-good-ticket>

# NERSC Consulting: What can you expect?

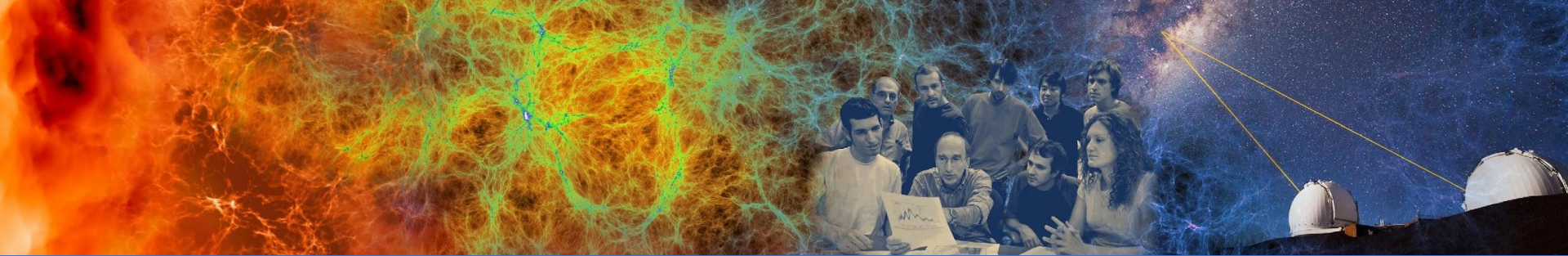
- Our first response will be within four business-hours
- We will help you resolve your problem, and keep you apprised of progress
- We welcome user feedback and constructive criticism

# NERSC User Appointments

- In 2018, we began offering “office hours”
  - Open Zoom meeting which users could join to get help with a particular topic, e.g., MFA, KNL Optimization, ERCAP, etc.
  - Shortcoming: long periods with no participants, then many jump on simultaneously
- Appointments: more efficient use of everyone’s time
- 30-minute appointments offered on a variety of topics:
  - GPU basics, Optimization, File Systems, Using GPUs in Python, Containers, NERSC 101, Checkpoint/Restart jobs with MANA, Spin, Appentra Codee
- Schedule an appointment: [nersc.as.me](https://nersc.as.me)

# NERSC Operations

- Operations staff are on site 24/7/365 to supervise operation of the machine room
- Operations know the health of the machines and can help users with some tasks (killing jobs, changes to running reservation, etc.)
- [NERSC MOTD](#) (message of the day, live status)
- Please avoid contacting Operations except in urgent cases



# Account Set Up



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**ENERGY**

Office of  
Science

# Accounts vs. Allocations

## There are two types of *accounts* at NERSC:

- Your personal, private, user account
  - Associated with your *login* or *username*
  - Provides *authentication* (personal identity) and *authorization* (which resources are accessible)
  - Five primary account *roles*
    - PI, PI Proxy, Project Membership Manager, Project Resource Manager, and User
- A Project allocation account, or *project*
  - Like a bank account you use to “pay” for computer time and file storage usage
  - Managed by a Principal Investigator (PI) and (optionally) one or more Project Managers.
  - All NERSC users belong to at least one project
  - An individual user may belong to more than one project
    - But only one *default project*

# Account Policies

- **All users must sign an Acceptable Use Policy form**
  - This is incorporated into the Self-Service account request form: <https://iris.nersc.gov/aup>
- **Password policies**
  - Must change password every year (365 days)
  - **Do not share passwords**
  - **Do not email passwords**
- **Account locked after 5 consecutive login failures**
  - Login to Iris to clear login failures
  - If you have forgotten your password, there is a link on the Iris login page that will lead you through the process of resetting a password
  - Email NERSC Account Support for more help



# Multi-Factor Authentication

- Provides an additional security layer to accessing NERSC
- Required for ALL users
- Generate a soft token
  - Link to a One-Time Password app/software
- Online instructions
  - <http://www.nersc.gov/users/connecting-to-nersc/mfa/>

# Iris - Web Based Information Portal

- **Web-based tool for user and project management**
  - Check daily balance, change password, change login shell, update contact information, etc.
  - Manage Project membership and allocations
  - Run reports

<https://iris.nersc.gov>

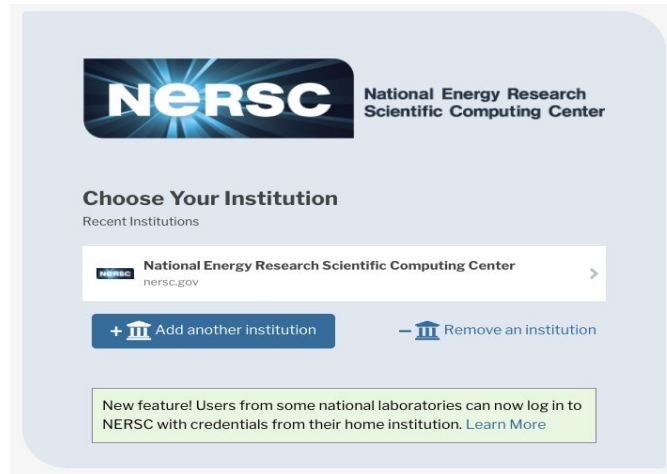
# Getting Help from the Iris Login Screen



The screenshot shows the Iris login interface. At the top center is the Iris logo, a sunburst icon with the word "Iris" in blue. Below the logo is the text: "Management and reporting for your account, compute and storage allocations, and projects at NERSC." A blue "Login" button is centered below the text. Underneath the button are three red text links: "Password Help", "Username Help", and "MFA Help". At the bottom of the screen, a light gray bar contains three red-bordered boxes with the text: "Forgot password?", "Forgot username?", and "MFA not working?".

# Federated Identity

- NERSC offers a Federated Identity option that allows you to log in with your current organization's credentials
  - Currently only available for some National Laboratories
  - <https://docs.nersc.gov/connect/federatedid/>



# Running Out of Time

- **User**

- PI determines how much of the project's computing allocation each user can use:
  - Either as a % of Total allocation or a fixed # of hours
- If user runs out of time
  - Submitted jobs go into the overrun queue if project cannot pay for job
  - Contact PI to increase percentage or # of hours

- **Project**

- If project runs out of time, PI should contact appropriate DOE Office of Science Program Allocations Manager
  - Each Program typically holds a certain amount of time in reserve
- Any jobs submitted will run in the overrun (low priority) queue

# User Responsibilities & Expectations

- Be kind to your neighbor users
  - Don't abuse the shared resources!
- Use your allocation smartly
  - Pick the right resource for your job and your data
- Back your stuff up
  - Especially from scratch, which has a purge policy
- Acknowledge NERSC in your papers
  - Acknowledge us so we can stay in business!
- Pay attention to security
  - Don't share your account with others!

Thank You and  
Welcome to  
NERSC!

