

Using NERSC Resources for College Courses in AI, Computational Science, & More!



Commonwealth Computational Summit
October 16, 2023

Rebecca Hartman-Baker, PhD
NERSC User Engagement Group Lead
rjhartmanbaker@lbl.gov

National Energy Research Scientific Computing Center

- NERSC is a national supercomputer center funded by the U.S. Department of Energy Office of Science (SC)
 - Supports SC research mission
 - Part of Berkeley Lab
- Researchers with funding from SC who need supercomputing resources can use NERSC
 - Other researchers can apply if research is in SC mission
- NERSC supports 10,000 users, 1,000 projects
 - From all 50 states + international; 60% from universities
 - Hundreds of users log on each day



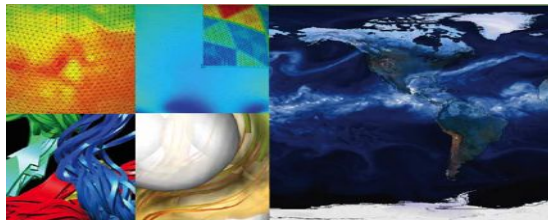
NERSC: Mission HPC for DOE Office of Science Research



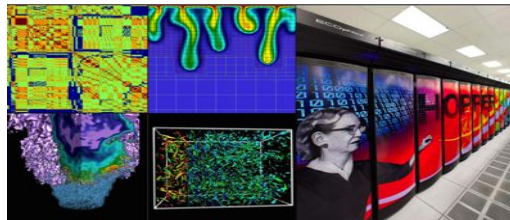
U.S. DEPARTMENT OF
ENERGY

Office of
Science

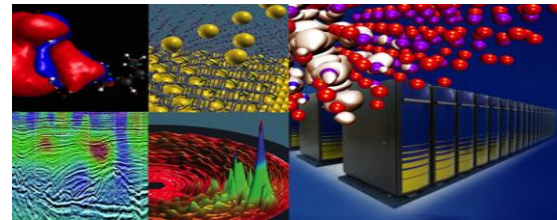
Largest funder of physical
science research in the U.S.



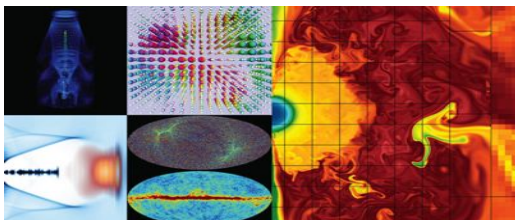
Biological & Environmental Research



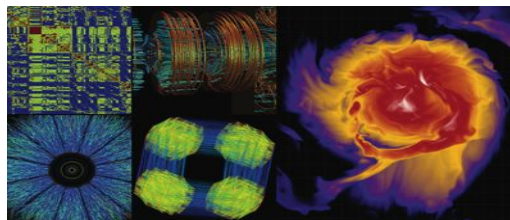
Computing



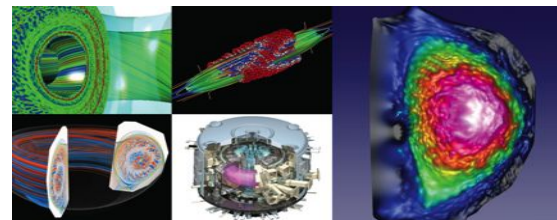
Basic Energy Sciences



High Energy Physics



Nuclear Physics



Fusion Energy, Plasma Physics



NERSC: Science First!

***NERSC's mission is to accelerate
scientific discovery
at the DOE Office of Science
through high-performance computing
and data analysis.***

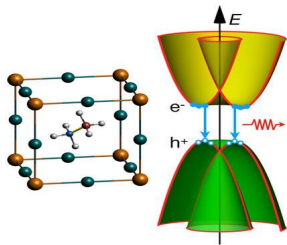


NERSC's Users Produce Groundbreaking Science

Materials Science

Revealing Reclusive Mechanisms for Solar Cells

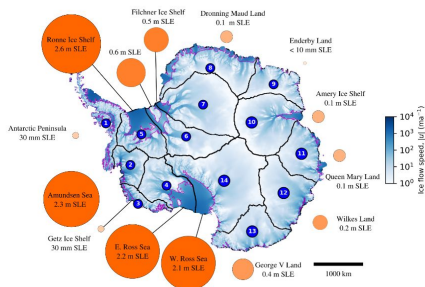
NERSC PI: C. Van de Walle, UC Santa Barbara, *ACS Energy Letters*



High Energy Physics

Shedding Light on Luminous Blue Variables

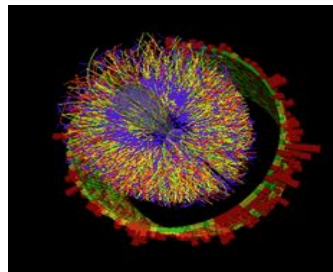
NERSC PI: Yan-Fei Jiang, UC Santa Barbara. *Nature*



Earth Sciences

Simulations Probe Antarctic Ice Shelf Vulnerability

NERSC PIs: D. Martin, Berkeley Lab; E. Ng, Berkeley Lab; S. Price, LANL. *Geophysical Research Letters*



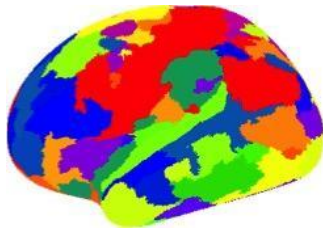
Nuclear Physics

Enabling Science Discovery for STAR

NERSC PI: J. Porter, Berkeley Lab. *J. Phys.: Conference Series*

Advanced Computing

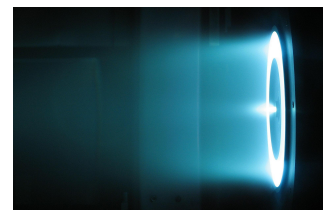
Scalable Machine Learning in HPC
NERSC PI: L. Oliker, Berkeley Lab, *21st International Conference on AI and Statistics*



Plasma Physics

Plasma Propulsion Systems for Satellites

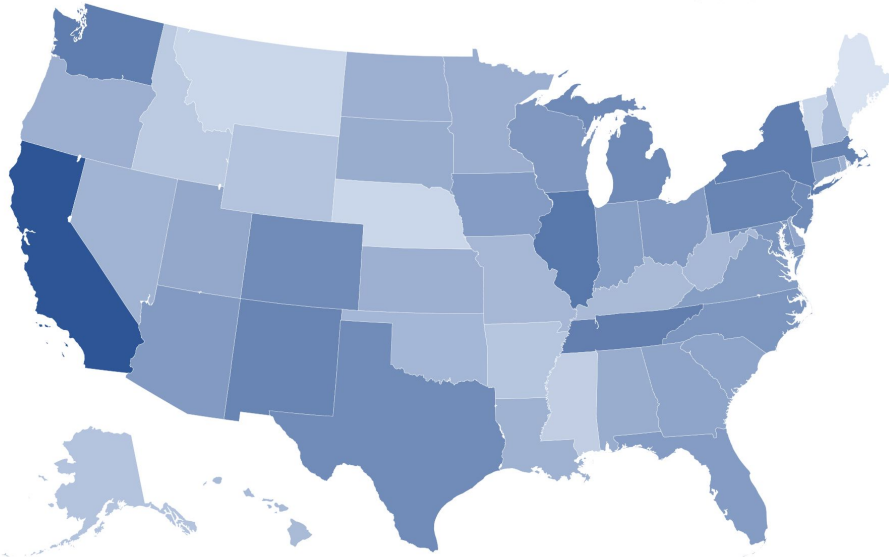
NERSC PI: I. Kaganovich, Princeton Plasma Physics Lab, *Physics of Plasmas*



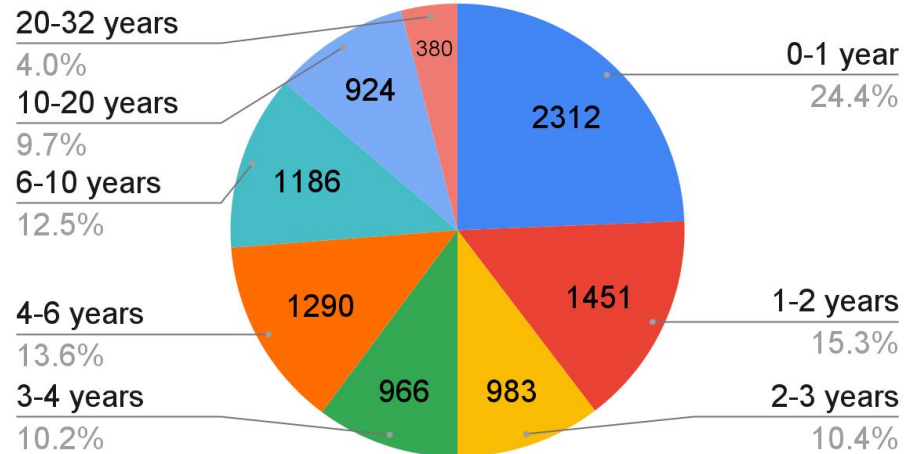
2,500 Refereed Publications per Year

NERSC Users Overview (2022)

Number of users (log scale) 
2 3414



Number of Users by Years as NERSC User



- 9,781 users across 1,083 projects
- Users from all 50 states plus international

- Majority < 3 years using NERSC
- Plurality of students

NERSC User Demographics

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



32%
Graduate
Students



19%
Postdoctoral
Fellows



15%
Staff
Scientists



13%
University
Faculty



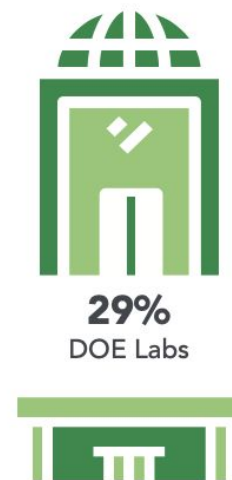
8%
Undergraduate
Students



5%
Professional
Staff



60%
Universities



29%
DOE Labs

5%
Other
Government Labs



4%
Industry



1%
Small
Businesses

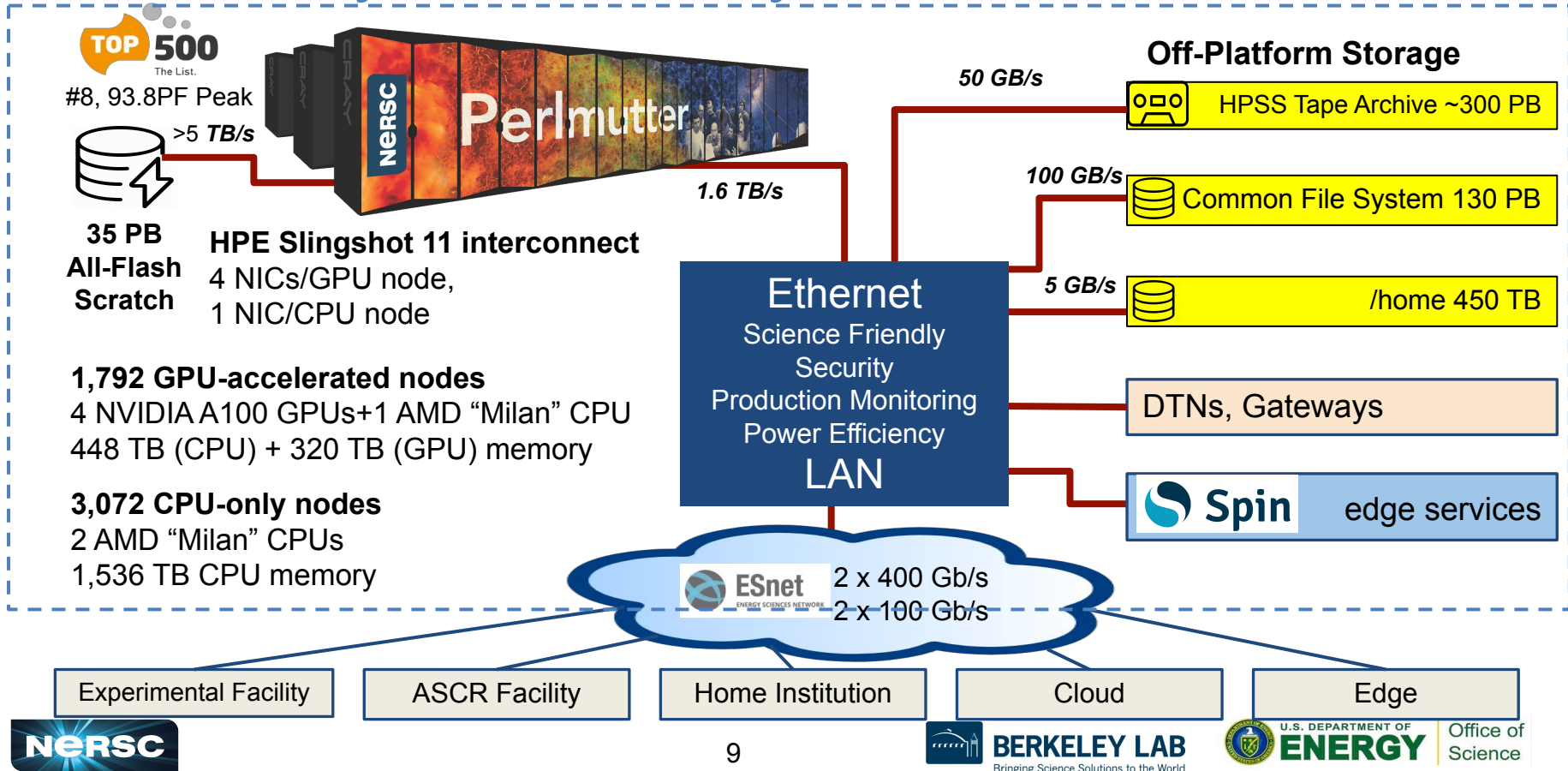


<1%
Private Labs

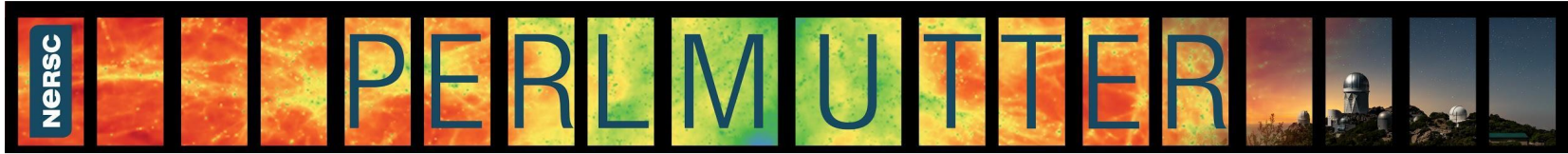
Kentucky Connections!

- 20 NERSC users from Kentucky institutions
 - 10 at UK, 6 at U of L, 3 at Centre College, 1 at Bellarmine University
- 4 NERSC projects with PIs in Kentucky
 - mp7: Lattice QCD Monte Carlo Calculation of Hadronic Structure and Spectroscopy (UK)
 - m3839: Understanding defect-driven reversible phase transitions in rare-earth nickelates for novel memory devices (U of L)
 - m3846: Atomic-scale understanding of ion conduction and interfacial processes in novel solid-state sodium batteries (U of L)
 - m4216: Improving Classical Molecular Dynamics Parameterization of Molecules for Battery Applications (Centre)

NERSC Systems Ecosystem



Perlmutter: Optimized for Science



- First phase arrived 2021; second phase in 2022; final acceptance in 2023
- GPU-accelerated and CPU-only nodes
- HPE Cray Slingshot high-performance network
- 35 PB all-flash scratch file system

GPU-Accelerated Nodes

- 1,536 GPU-accelerated nodes
- 1 AMD “Milan” CPU + 4 NVIDIA A100 GPUs per node
- 256 GB CPU memory and 40 GB GPU high BW memory

CPU-Only Nodes

- 3,072 CPU only nodes
- 2 AMD “Milan” CPUs per node
- 512 GB memory per node

HPC Systems: Perlmutter

GPU nodes:

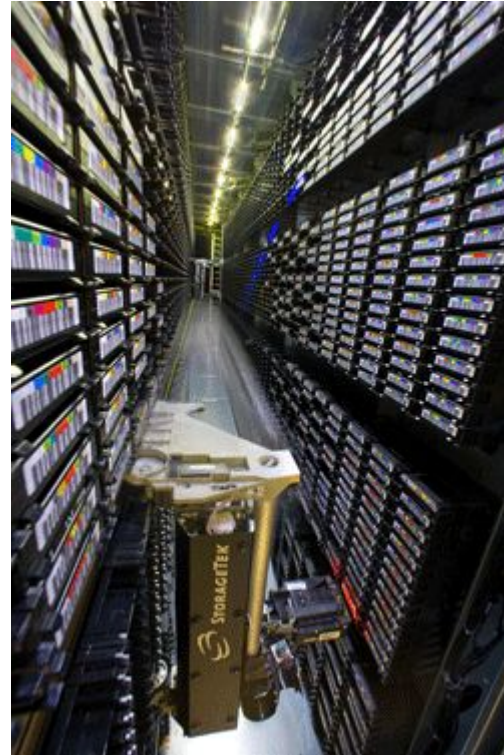
- Immense compute power from GPUs
- Large jobs using many GPUs encouraged
- Great for codes that can exploit GPU compute power

CPU nodes:

- Powerful CPUs (but only 10% of GPU compute power)
- Equivalent in compute power to all of Cori (former system)
- More like a traditional cluster
- Great for throughput jobs

File Systems

- Global File Systems:
 - Home
 - Community (CFS)
- Local File Systems:
 - Scratch
- Long-term Storage System:
 - HPSS



Global File Systems

Home

- Permanent, relatively small storage
- Mounted on all platforms
- NOT tuned to perform well for parallel jobs
- Quota cannot be changed
- Snapshot backups (7-day history)
- **Perfect for storing data such as source code, shell scripts**

Community File System (CFS)

- Permanent, larger storage
- Mounted on all platforms
- Medium performance for parallel jobs
- Quota can be changed
- Snapshot backups (7-day history)
- **Perfect for sharing data within research group**

Local File Systems

Scratch

- Large, temporary storage
- Local to machine
- Optimized for read/write operations, NOT storage
- Not backed up
- Purge policy (12 weeks)
- **Perfect for staging data and performing computations**



Long-Term Storage System

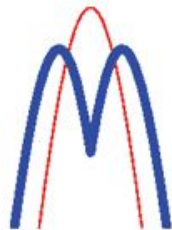
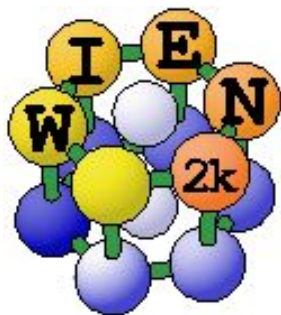
HPSS

- High-Performance Storage System
- Archival storage of infrequently accessed data
- Hierarchical storage:
 - Data first ingested onto high-performance disk arrays
 - Migrated to large enterprise tape subsystem for long-term retention

NERSC Provides a Diverse Software Ecosystem

- HPE Cray supercomputer OS is a version of Linux
- Compilers are provided on machines
- Libraries: many libraries are provided by vendor, still others provided by NERSC
- Applications: NERSC compiles and supports many software packages for our users

Chemistry & Materials Science Applications



Molpro



QUANTUM ESPRESSO



BerkeleyGW

abinit.

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



NAMD

Scalable Molecular Dynamics



GÅMESS

LAMMPS

WANNIER90

CPMD



NWCHEM

HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE



NERSC has a rich data ecosystem!



data transfer and access



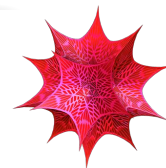
mongoDB®



data management



julia



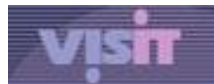
data analytics



PyTorch



machine learning



ParaView
Parallel Visualization Application

visualization



SHIFTER

Spin

containers



GNUparallel



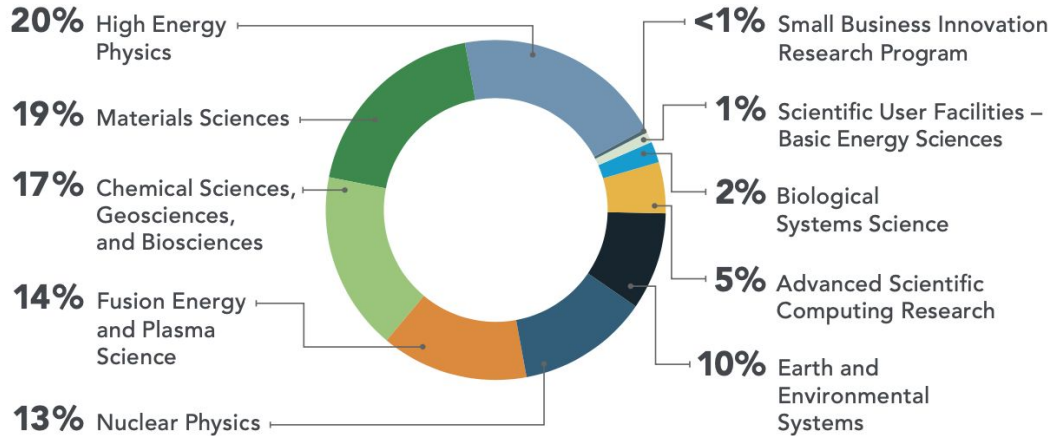
papermill

workflows



Compute Hours Breakdown

Breakdown of Compute Used by DOE Program

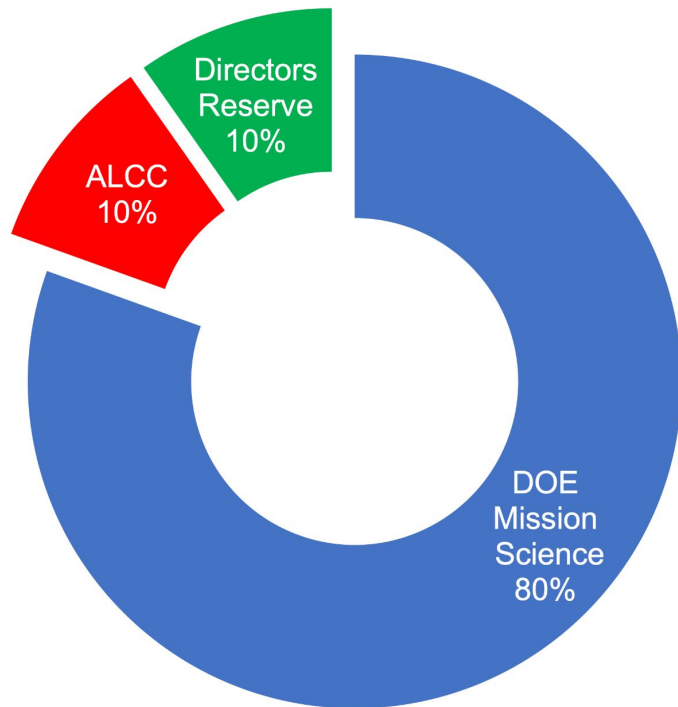


Top Science Disciplines

(By computational hours used)



Allocation Programs



Distributed by DOE Office of Science program managers

Competitive awards run by DOE Advanced Scientific Computing Research Office

Strategic awards from NERSC

NERSC doesn't pick most users; they are chosen by DOE Office of Science allocation managers

Director's Reserve Includes Education Allocations

- NERSC supports instructors with educational allocations
- You can apply for an allocation for a course you are teaching, even if you are not already a NERSC user
- Apply about 6-8 weeks before resources are needed through the ERCAP system (ercap.nersc.gov)

NERSC Education Project Steps & Lifecycle

1. If you don't have an existing account, apply for an ERCAP submission account
2. Fill out and submit the ERCAP project application form
3. If successful, have your students apply for user accounts in your project

Applying for an ERCAP Submission Account

- If you have an existing NERSC account, use that
 - Even if it is inactive, we can “revive” your old account and give you access to it
 - Reactivate your old account by sending an email to accounts@nersc.gov
- If you do not have a NERSC account, apply for a new NERSC PI account at: <http://iris.nersc.gov/add-pi>
 - It could take 1-2 business days, so plan ahead!
 - You will receive an email when your account is ready

New PI Request Form



Create a New NERSC PI Account

Requested Username ⓘ ⓘ
Username must be 3 to 8 characters long, must start with a letter and may not be a common unix command.

First Name ⓘ ⓘ

Middle Name

Last Name ⓘ

Citizen Of ⓘ ▾ **Have Greencard?**

Select an organization
Please select a valid organization.
[I can't find my organization](#) ←

Email ⓘ

Work Phone ⓘ
Please enter a valid phone number

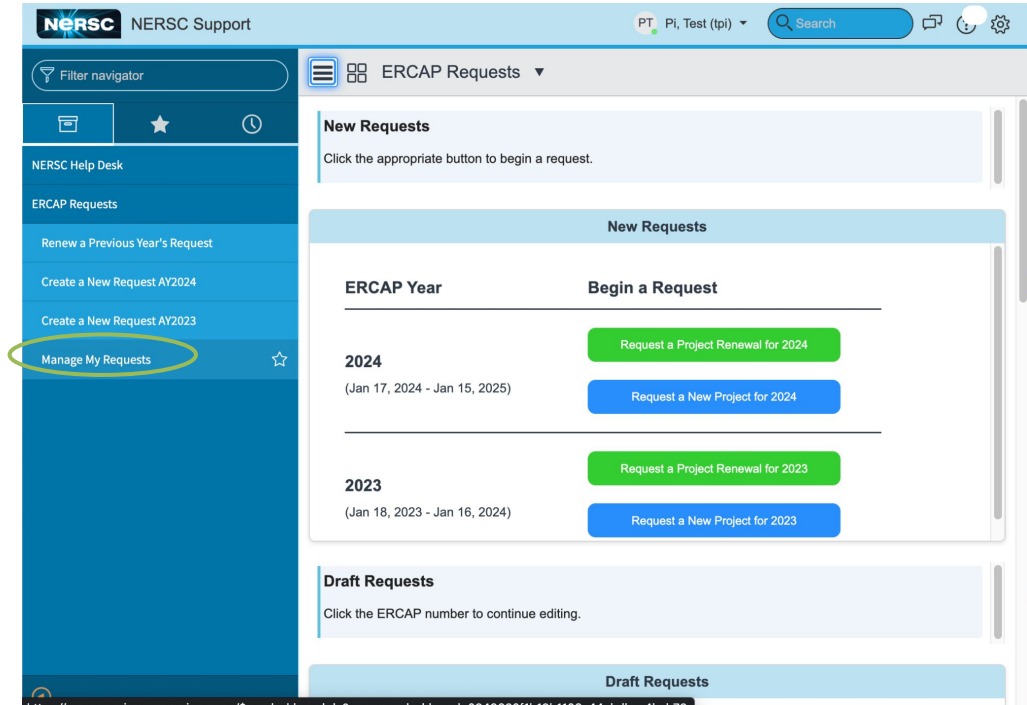
⊙ OK

⊖ Cancel

There are thousands of organizations in our database, but if yours is not there, you can add the organization via this link

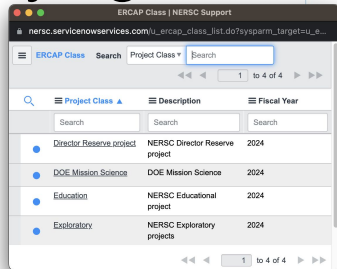
ERCAP Project Request Form: Getting Started

- Navigate to <https://ercap.nerisc.gov>
- Log in, and select “Manage My Requests” from side menu
- Click on blue “Request a New Project” for appropriate year



ERCAP Project Request Form: Overview

- Gray boxes mean info not editable
- **Red stars** indicate required info that needs to be filled in before submitting form
- Search for choices by clicking magnifying glass; a small window pops up



The screenshot shows the "ERCAP Requests - ERCAP0029395" form. At the top, there's a navigation bar with "PT Pi, Test (tpi)", a search bar, and icons for help and settings. Below that, a breadcrumb trail shows "Draft" > "Submitted for Review" > "Approved" > "Provisioned".

A blue box contains instructions: "Click the magnifying glass icon to select from a list.", "Place the mouse over any label text for a description of what to enter.", "The asterisks (*) next to labels and in the tabs indicate there is information that is mandatory for the request.", and "To submit a renewal, click the 'This request is a renewal' checkbox below."

The form fields include:

- "This request is a renewal." checkbox (unchecked)
- "ERCAP Number" field: ERCAP0029395 (grayed out)
- "* Project Title" field: empty
- "* Label" field: empty
- "* PI Name" field: Pi, Test (tpi) (with magnifying glass icon)
- "Allocation Year" field: 2024 (grayed out)
- "State" field: Draft (grayed out)
- "* Project Class" field: DOE Mission Science (with magnifying glass icon)
- "* Program" field: empty (with magnifying glass icon)
- "* Science Category" field: empty (with magnifying glass icon)
- "Project" field: empty (grayed out)

At the bottom, there are tabs for "Personnel", "Funding*", "Security*", "Project Details*", "Resources*", "Codes*", "Supporting Information*", and "Usage Agreement*".

Below the tabs, there's a text input field for "Senior" with the instruction: "Enter the name, organization, and email address of Senior Investigators or Key Personnel you would like to have associated with your project."

ERCAP Project Request Form: Overview

For Project Class, select “Education”

For Program, select “NERSC DDR - NERSC Education”

For Science Category, select your science area from the list

ERCAP Number	<input type="text" value="ERCAP0029395"/>	Allocation Year	<input type="text" value="2024"/>
* Project Title	<input type="text" value="Test Education Project"/>	State	<input type="text" value="Draft"/>
* Label	<input type="text" value="test_ed"/>	* Project Class	<input type="text" value="Education"/> <input type="button" value="Q"/> <input type="button" value="i"/>
* PI Name	<input type="text" value="Pi, Test (tpi)"/> <input type="button" value="Q"/> <input type="button" value="i"/>	* Program	<input type="text" value="NERSC DDR - NERSC"/> <input type="button" value="Q"/> <input type="button" value="i"/>
		* Science Category	<input type="text" value="Energy : Fusion"/> <input type="button" value="Q"/> <input type="button" value="i"/>
		Project	<input type="text"/>

ERCAP Project Request Form: Tabs

Multiple tabs with required information

Personnel	Funding*	Security*	Project Details*	Resources*	Codes*	Supporting Information*	Usage Agreement*
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Most info is straightforward

ERCAP Project Request Form: Personnel

Personnel Funding* Security* Project Details* Resources* Codes* Supporting Information* Usage Agreement*

Enter the name, organization, and email address of Senior Investigators or Key Personnel you would like to have associated with your project.

Senior Investigators

Click on the magnifying glass below to search for existing NERSC users. Then, choose a name to add your selection to the list of authorized preparers for this request. If you would like to add a preparer who is not a NERSC user, please have that person fill out [this form](#) and include in the Comments that they are an Authorized Preparer for you as the PI.

Authorized Preparers

Select target record

List additional instructors (if any) as Senior Investigators. Optionally add another person authorized to prepare the request

ERCAP Project Request Form: Funding

Personnel Funding* Security* Project Details* Resources* Codes* Supporting Information* Usage Agreement*

What entity(ies) fund the research associated with this request? Check all that apply.
You must select the primary funding source before you can submit your request.

* Primary Funding Source

DOE Office of Science (SC)

Federal Agency other than DOE/SC

LDRD Funding

State or local government or agency

Foreign Government or Agency

University

* University name and grant numbers

Primary funding source is your college or university

Scroll to bottom of Funding page to answer question about relevance to DOE

For projects not funded by DOE/SC, please describe the project's relevance to one of the [DOE Office of Science programs and the mission of that program](#).
(Projects that can demonstrate alignment with a program mission are much more likely to receive awards.)

* Office of Science relevance

ERCAP Project Request Form: Security

NERSC does not allow proprietary or export controlled research or data on its systems. Select “I attest...” to agree to avoid these in your education project

Personnel	Funding	Security*	Project Details*	Resources*	Codes*	Supporting Information*	Usage Agreement*
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NERSC supports only open research intended to be published in open scientific journals. Proprietary research is not allowed.

In addition, NERSC does not allow the use of the following:

- **Classified or controlled military defense information**
- **Export controlled or ITAR codes or data**
- **Personally identifiable information**
- **Protected health information**

Please select one option below:

* I attest that this project adheres to these guidelines.

* I request an exception to these policies, based on the following:

* Please Explain Policy Exception

ERCAP Project Request Form: Project Details

Write a summary & a more detailed overview of your plans. 5-10 sentences at most

Renewal requests must provide additional info below

Project

Personnel Funding Security **Project Details*** Resources* Codes* Supporting Information* Usage Agreement*

To attach a supporting document, click the paperclip icon at the top of the page. When done, click the X to close the window.

Provide a brief summary of your project easily understood by people outside your field. What will this project accomplish? What is the significance of this work?

* Project Summary and Goals

Provide a more technically detailed explanation of your research for proposal reviewers.

* Detailed Description for DOE Managers

Enter a URL for a relevant web page describing your project. Enter ONLY ONE URL per line using the format: http://www.nersec.gov

Website URL

Provide the information below for **Renewal requests** only.

ERCAP Project Request Form: Resources

Personnel	Funding	Security	Project Details	Resources	Codes*	Supporting Information*	Usage Agreement*
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Computational Resources - Enter the number of NERSC computational hours requested.

CPU Node Hours Used	<input type="text" value="0"/>	* CPU Node Hours Requested	<input type="text" value="1,234"/>
GPU Node Hours Used	<input type="text" value="0"/>	GPU Node Hours Requested	<input type="text" value="5,678"/>

If you are applying for GPU time, please tell us about your code's [readiness](#) to use GPUs.

* GPU Readiness	<input type="text" value="Our code, cool_science, has been ported to GPUs. Others have run the code on up to 1024 NVIDIA GPUs."/>		
What is the typical number of nodes your individual jobs will use concurrently?	<input type="text" value="1"/>	What is the maximum number of nodes your individual jobs could use concurrently?	<input type="text" value="20"/>

Briefly describe how you estimated the compute hours requested above as a justification for the Reviewers to determine the appropriateness of your request.

* Justification for Compute Request	<input type="text" value="We estimate that each student in the 25-person class will use approximately 20-50 CPU node-hours and 50-100 GPU node-hours on their final project, in addition to day-to-day course exercise usage"/>
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Estimate the number of node-hours required, explain GPU readiness (if applicable), and justify the overall compute-hour request

Scroll down to answer more questions about disk space and utilization patterns

ERCAP Project Request Form: Codes

List any libraries or software required and describe up to 5 codes that your project is using

Personnel	Funding	Security	Project Details	Resources	Codes	Supporting Information *	Usage Agreement *
Please list the 3rd party or community software packages (eg. math libraries) that you need NERSC to provide.							
Software Dependencies		PETSc, FFTW, HDF5, cmake					
If you are NOT planning to run any codes, enter N/A in the code name box and briefly explain what NERSC resources you will be using in the code description box. (Please list the application codes or frameworks you will run at NERSC.)							
How many codes will you use? (select up to 5)		1					
* Code 1 Name		cool_code					
Code 1 URL		www.cool-code.org					
* Code 1 Description		This code is really cool. It can simulate anything.					
Code 1 is GPU Enabled?		<input checked="" type="checkbox"/>					

ERCAP Project Request Form: Supporting Info

Are you using other HPC resources? If so, describe

Personnel	Funding	Security	Project Details	Resources	Codes	Supporting Information*	Usage Agreement*
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List any additional HPC resources that have been awarded or are expected to be used to support this project.

* Other HPC Support

Supply any other additional information you would like to be considered in support of this request.

Additional Information

To attach a supporting document, click the paperclip icon at the top of the page. When done, click the X to close the window.

Use this space to provide feedback on ERCAP, the NERSC application/allocation process.

Feedback

Save as Draft Create PDF Submit for Review

ERCAP Project Request Form: Usage Agreement

Personnel	Funding	Security	Project Details	Resources	Codes	Supporting Information	Usage Agreement*
-----------	---------	----------	-----------------	-----------	-------	------------------------	------------------

If this project is given a NERSC award, I agree to monitor the usage associated with it to ensure that, to the best of my ability, usage is for the project described here. Furthermore, if this is a continuing project, I confirm that I have audited the usage associated with this project, and to the best of my ability to determine, all usage was for the project described here and users are adhering to the [NERSC Appropriate Use Policies](#).

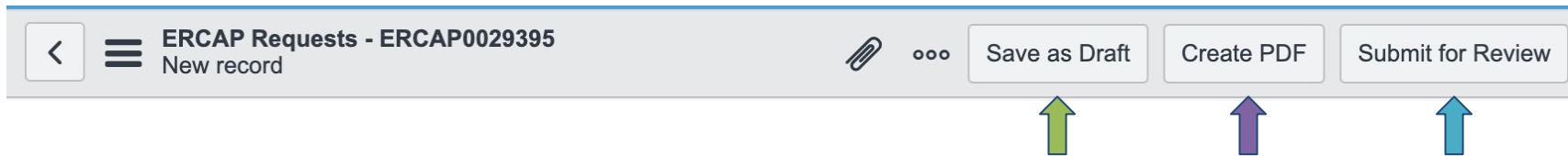
By signing this application, I certify that the statements herein are true, complete and accurate to the best of my knowledge. I also agree to comply with any resulting terms if I accept an award. (<https://www.nersc.gov/users/policies/>). I am aware that any false, fictitious, or fraudulent statements or claims may subject me to criminal, civil, or administrative penalties. (U.S. Code, Title 18, Section 1001)

Please enter your initials below to agree to these terms.

* Usage Agreement Initials

Initial to indicate your agreement with NERSC's Terms and Conditions

ERCAP Project Request Form: Saving & Submitting



At any time you can **save a draft**, **create a PDF** of your request, or **submit request for review**

Requests will be evaluated and resourced within 4-6 weeks (or at beginning of allocation year if requesting for next allocation year)

Resources

- Getting an Allocation
 - [Apply for your first NERSC allocation](#)
 - [The NERSC Allocation Request Form](#)
- Managing a Project
 - [Managing your allocation and your users](#)
 - [Iris Guide for PIs and project managers](#)