NUG Monthly Meeting

14 December, 2023

Today's plan

- Interactive - please participate!
  - **NERSC User Slack** (link in chat)
  - **#webinars** channel

- Agenda:
  - Holiday ICE Breakers - NERSC Edition
  - General NERSC Updates/Announcements
  - Calls for Participation
  - Upcoming Scheduled Trainings
  - NERSC Allocation Year Transition (UEG, Helen He)
  - Current NERSC HPC Training Strategy (UEG, Helen He)

HOLIDAY ICE Breakers

- What is your favorite Christmas/Holiday gift that you have every received and why?

Holiday Ice Breaker - Favorite Gift?

- What is your favorite annual holiday tradition or activity?

- What is your most important goal or New Year's Resolution for 2024 and why?

Announcements - NERSC Updates

- (NEW/UPDATED) Allocation Year 2024 Begins January 17, 2024!
- 2024 ERCAP Allocations Announced Later this Week
- DOE-SC Annual User Stats Call
- NERSC Shell Support Policy
- Changes to Science Gateways using PHP at portal.nersc.gov

Reminder: Please see the Weekly Email for Links!

Announcements - Calls for Participation

- Nominate a Colleague for the James Corones Award in Leadership, Community Building, & Communication by December 31
  - recognizes mid-career scientists/engineers making an impact in leadership, community building, or science communication.
- Applications for DOE Computational Science Graduate Fellowship Now Open! (Due Jan 17, 2024)

Reminder: Please see the Weekly Email for Links!

Announcements - Meetings/Trainings

- Kokkos User Group Meeting December 12-15
  - being held 12th through 15th of December 2023 in Albuquerque, NM
- Applications Now Open for E3SM Tutorial Workshop
  - The E3SM project, supported by the US Department of Energy's (DOE's) Biological and Environmental Research (BER) Earth and Environmental Systems Sciences Division (EESSD) and Earth System Model Development (ESMD) programs will hold its first in-person tutorial workshop at NERSC, May 7-10, 2024.
  - The tutorial will include:
    - Lectures on earth system simulation and the model components of E3SM.
    - Practical sessions on running E3SM, modifying components, and analyzing data.
    - Best practices for utilizing the model and potentially contributing to its development.

Reminder: Please see the Weekly Email for Links!

Announcements - Scheduled Outages

Please see the Weekly Email for Links!

- **Perlmutter**
  - 12/20/23 06:00-22:00 PST, Scheduled Maintenance
  - 01/17/24 06:00-22:00 PST, Scheduled Maintenance
- **HPSS Regent (Backup)**
  - 12/13/23 09:00-13:00 PST, Scheduled Maintenance
    - Some retrievals may be delayed during tape drive firmware update.
  - 01/03/24 09:00-13:00 PST, Scheduled Maintenance
    - HPSS will be available while we upgrade Library firmware. Some retrievals may be delayed during tape library maintenance.

https://www.nersc.gov/live-status/motd/

Allocation Year Transition

Helen He, UEG

Outline
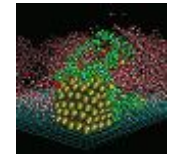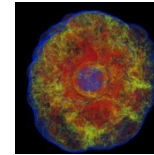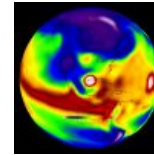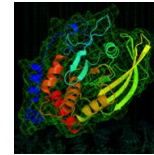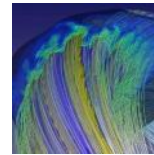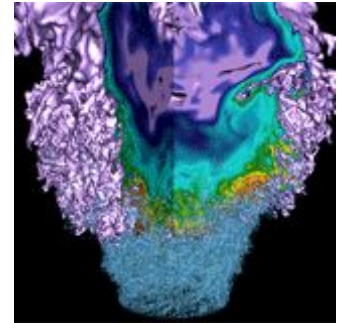
- AY2024 Allocations

- AY Transition Process

- On the AY2024 Start Day

- Changes in AY2024

- Discontinued Users

AY2024 Allocations

- AY2024: Wed, Jan 17, 2024 - Tue, Jan 14, 2025
- AY2023 allocation hours do not carry over
- Allocation award emails go out the week of Dec 11
- Each project has separate CPU and GPU awards
- AY2024 charge starts on Thur, Jan 18

What Happens at AY Transition?

- Iris needs to be updated with the new AY2024 allocation data: projects, users, CPU, GPU and HPSS storage allocations awarded, etc.

- Computational systems need to sync up with the Iris active users data and clean up batch jobs that do not have AY2024 allocations

- System maintenances

- Some other changes: policy, software, ...

- More information at
  https://www.nersc.gov/allocation-year-transition-2023-to-2024/

Shortly before AY2024 starts …

- No new user account creation/validation: Jan 10-16, 2024

- No new AY2023 project requests (via ERCAP) after Oct 3, 2023

- Before end of AY2023 (deadline is Jan 12, 2024)
  - PIs must select which users will continue in project in AY2024
  - PIs must check/update which users will have "premium" QOS access for AY2024
    - Previous year's allowed list is inherited
  - Instructions at:
    https://docs.nersc.gov/iris/iris-for-pis/#set-your-user-list-for-the-next-allocation-year   (API in IRIS via "Roles" tab for this feature will be available soon)

On the AY2024 Start Day, Jan 17 (1)

- **Iris:** Downtime: 7 am - 9:30 am
  - Logout and login to reflect new AY data
- **Perlmutter**: Scheduled maintenance 6 am - 10 pm
  - Login and compute nodes availability info will be provided later
- **Jupyter**
  - Access may be impacted depending on Perlmutter status, such as login and compute nodes availability
- **All other systems and services are up**

On the AY2024 Start Day, Jan 17 (2)

These jobs will be deleted on Perlmutter

- Jobs associated with non-continuing projects
- Jobs associated with a continuing project that the user is no longer a member of AY2024
- "overrun" jobs
- Held jobs older than 12 weeks

After AY2024 Starts

- **PIs should check/update CPU and GPU allocations allowed for each user in Iris once AY24 starts**
  - Percentages allowed for each user are inherited from last year
  - Hours allowed for each user are **NOT inherited** from last year
    - The reason behind this is some users have a huge number inherited previously from before the unit was based on Perlmutter hours
  - Percentage takes precedence over hours if both are set

New Appropriate Use Policy

- NERSC's Appropriate Use Policy is being updated for AY24 to better reflect the way that NERSC resources are used by the NERSC user community.

- All users are required to agree to the updated policy

- More details will be provided later for the process

Discontinued Users

- Users with no active project are "discontinued", effective AY2024 starts on Jan 17, 2024
- Can login to authorized systems (Perlmutter, HPSS, DTN, etc.) for 60 days until Mar 16, 2024 for data access, but can not run batch jobs
  - Clean up and transfer files back to their home institutions
- Detailed policy at https://docs.nersc.gov/accounts/policy/#account-deactivation-process

NERSC User Training
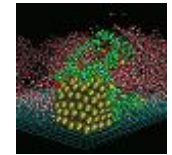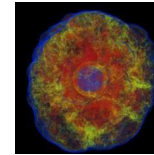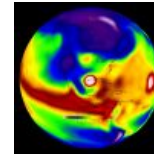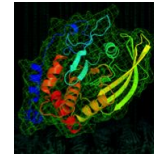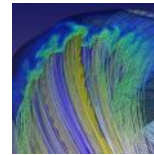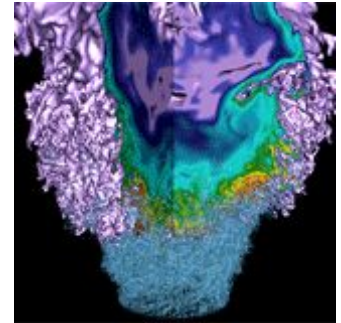
Helen He, UEG

Outline

- Training Team, Goals, and Strategy
- Achievements
- Current State of the Art
- Future Planning

Core Training Team

Strategic planning, initiating, and soliciting

Helen He   Lipi Gupta   Charles Lively   Shashank Subramanian

with contributions by numerous NERSC staff from each group
and our collaborations with other HPC centers and vendors

Training Goals

- Provide knowledge to our users on Resource Familiarization, Optimized Utilization, and Skills Development for effectively using NERSC resources
- Examine user personas and synthesize with plans for Perlmutter and future systems to help determine training strategy
  - Personas: different profiles of user types (e.g., novice, advanced, data, simulation, PIs, etc.)
  - Training topics: informed by user personas to provide comprehensive training

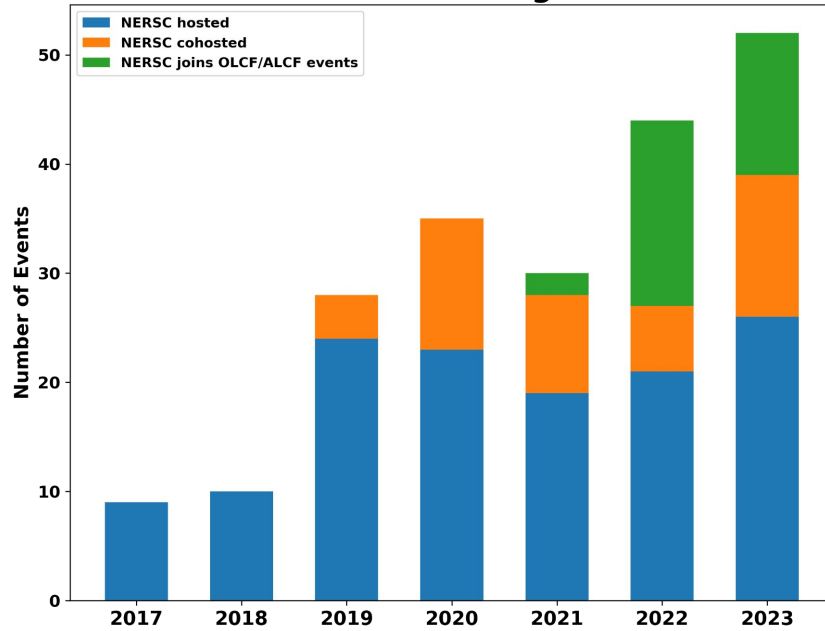# Considerations in Strategic Planning

- User need
- User impact
- User technical levels and personas
- Learning styles
- Staff resources
- Collaboration with other HPC centers (OLCF/ALCF, etc.)
- Collaboration with vendors and developers

4-5x Increase in Number of Training and Attendees since 2018

Number of Training Events

Number of Training Attendees
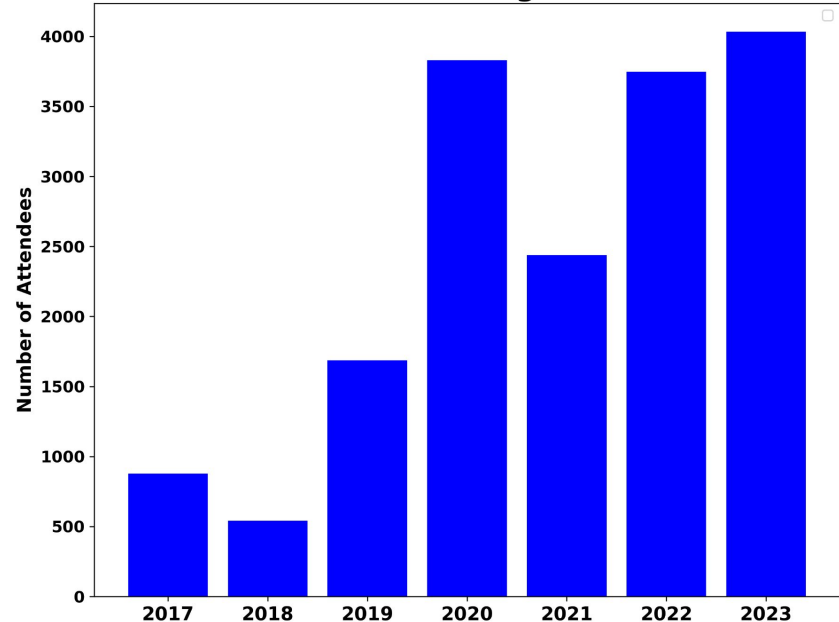
Expanding Depth & Breadth of Offerings

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Events	Data User, Novice	Simulation User, Novice	Data User, Advanced	Simulation User, Advanced	PIs	Vendors	DOE/NERSC Leadership
CUDA to SYCL Migration				✅		✅	
BerkeleyGW Tutorial and Conference		✅					
Migrating from Cori to Perlmutter (5)	✅	✅	✅	✅			✅
N-Ways to GPU Programming Bootcamp		✅		✅		✅	
Workflow Software Across DOE Facilities	✅			✅			✅
Codee Training		✅					
SpinUp Workshops (4)			✅		✅		
Julia Training	✅		✅				
Advanced SYCL Training				✅		✅	
NERSC: Scientific Discovery through Computation	✅	✅			✅	✅	✅
Intro to NERSC Resources	✅	✅	✅	✅			
Crash Course in Supercomputing		✅		✅			
LaTex Workshop	✅	✅	✅	✅	✅	✅	
Modern Fortran Basics		✅		✅			
ALCF SambaNova AI Woskshop	✅		✅			✅	
OLCF AI Training Series (3)	✅	✅	✅	✅			

Training Coverage across Stakeholder Personas (2)

Events	Data User, Novice	Simulation User, Novice	Data User, Advanced	Simulation User, Advanced	PIs	Vendors	DOE/NERSC Leadership
NERSC GPU Hackathon	✓	✓	✓	✓		✓	
Quantum Computing Training (2)			✓	✓	✓	✓	
ALCF Graphcore AI Training	✓		✓				
ECP UPC/CoarrayFortran/Chapel		✓	✓	✓			
Intro to HPC Bootcamp	✓	✓			✓		✓
HIP Training Series (5)		✓		✓	✓	✓	
OLCF Frontier Training Workshop		✓	✓	✓	✓	✓	
New User Training	✓	✓	✓	✓	✓		
Writing an Effective ERCAP Proposal	✓	✓	✓	✓	✓		✓
NERSC SF API	✓	✓	✓	✓	✓	✓	
OpenMP Offload (4)		✓		✓		✓	
Raja Training		✓		✓		✓	
NERSC End-to-End AI for Science Bootcamp	✓	✓	✓	✓			
GPUs for Science Day	✓	✓	✓	✓	✓	✓	✓
Quantum Day	✓	✓	✓	✓	✓	✓	✓
Data Day	✓	✓	✓	✓	✓	✓	✓
HPE CPE and Optimization on GPUs		✓	✓	✓	✓	✓	

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Offering Variety of Topics

Using Systems	Programming Models and Tools	Applications	Data Analytics	Other
Migrating from Cori to Perlmutter	CUDA to SYCL Migration	BerkeleyGW Tutorial and Conference	Workflow Software Across DOE Facilities	SpinUp Workshops
Intro to NERSC Resources	N-Ways to GPU Programming Bootcamp	NERSC GPU Hackathon	Julia Training	NERSC: Scientific Discovery through Computation
OLCF Frontier Training Workshop	Codee Training	GPUs for Science Day	ALCF SambaNova AI Training Workshop	LaTex Workshop
New User Training	Advanced SYCL Training		ALCF Graphcore AI Training	Quantum Computing Training
Using Perlmutter	Crash Course in Supercomputing		NERSC SF API	Intro to HPC Bootcamp
	Modern Fortran Basics		NERSC End-to-End AI for Science Bootcamp	Writing an Effective ERCAP Proposal
	ECP UPC/Coarray Fortran/Chapel			Quantum Computing Training
	HIP Training Series			Quantum Day
	OpenMP Offload			
	Raja Training			
	HPE CPE and Optimization on GPUs			

Sample User Pathways (1)

- **Novice Data User => Advanced Data User**
  - New User Training
  - Using Perlmutter
  - Data Day
  - Workflows software
  - AI for Science Bootcamp
  - GPU Hackathon
  - GPUs for Science Day

Sample User Pathways (2)

- Novice Simulation User => Advanced Simulation User
  - New User Training
  - Migrating from Cori to Perlmutter Training
  - N-ways to GPU Programming Bootcamp
  - OpenMP Offload
  - Modern Fortran Basics
  - Codee Training
  - HPE CPE and Optimization on GPUs
  - GPU Hackathon
  - GPUs for Science Day

Exploring New Scopes

- ## Intro to HPC Bootcamp
  - Outreach to minorities community
  - Collaboration among multiple DOE labs and Sustainable Horizon Institute (SHI)
  - Workforce development for next generation HPC professionals
- ## NERSC Users pre-HPC training
  - Basic computing knowledge
  - Establish solid foundation prior to using NERSC HPC systems

SYSTEMS   FOR USERS   NEWS   R & D   EVENTS   LIVE STATUS

Home » News » News » Center News » DOE's First 'Intro to HPC' Bootcamp Focuses on Energy Justice and a New Model for Workforce Development

DOE'S FIRST 'INTRO TO HPC' BOOTCAMP FOCUSES ON ENERGY JUSTICE AND A NEW MODEL FOR WORKFORCE DEVELOPMENT

Broad-based program emphasizes social issues to attract a diverse pool of students to computing sciences

SEPTEMBER 13, 2023
By Kathy Kincade
Contact: cscomms@lbl.gov

Energy justice and workforce development were the driving themes of the US Department of Energy's (DOE's) first "Introduction to High-Performance Computing (HPC) Bootcamp," held at Lawrence Berkeley National Laboratory (Berkeley Lab) August 7-11 and hosted by the National Energy Research Scientific Computing Center (NERSC), in collaboration with the Argonne Leadership Computing Facility (ALCF), the Oak Ridge Leadership Computing Facility, and the Sustainable Horizons Institute (SHI). The event was funded by the DOE's Exascale Computing Project (ECP).

Participants in the DOE's Introduction to High-Performance Computing Bootcamp pose together at Berkeley Lab. (Credit: Berkeley Lab)
Select the image [offsite link ↗] to view more photos.

Exploring New Scopes: LMS

- Learning Management System (LMS)
  - Centralized access to learning materials and resources
  - User management for trainers and learners
  - Asynchronous training modules at different leve
  - Assessment and progress tracking capabilities
  - Certification system (possibly a required test)
- **CANVAS LMS** currently under Evaluation
  - https://www.instructure.com/canvas/

Longer Term Planning Strategy

- Align with NERSC strategic goals on N9 and N10
  - Perlmutter (N9) has Simulation and Data users. GPU is a focus
    - Continue to move workload to GPUs
    - Programming models, Using systems, Applications
    - Portability series
  - N10 has more integrated workflow requirement
    - Support IRI and AI/Learning workloads
    - Workflows, SPIN, Superfacility, Containers
- Again, consider user need, user impact, user technical levels and personas, learning styles, staff resources, collaborations, etc.

Ongoing Training Ideas with Strategic Goals

GPUs / Portability	IRI / Workflows	AI / Learning	Containers	HPC Pipeline
New User Training	New User Training	New User Training	New User Training	Intro to HPC Bootcamp
Intro to NERSC Resources	Workflows Software	DASK	Podman Training	pre-HPC Trainings
Using Perlmutter / N10	Using Perlmutter / N10	RAPIDS Bootcamp	Using Perlmutter / N10	Quantum Computing Training
OpenMP Training Series	SPIN	Deep Learning at Scale Tutorial	Containers Tutorial	Quantum Day
Nvidia Compilers and Tools	Data Day	Using Perlmutter / N10		Writing an Effective ERCAP Proposal
N-ways to GPU Programming	Superfacility API	AI Frameworks		
Portability Series: Kokkos, HIP, SYCL, AMRex, HPX, ...	Julia	Data Day		
Codee Training		GPUs for Science Day		
GPU Hackathon		AI for Science Bootcamps		
GPUs for Science Day		Julia		
MPI Training				
Fortran, C++ Trainings				
Applications and Domain Science Areas: BerkeleyGW, VASP, E3SM...				

Links to Training Materials and Planning

- Training Upcoming Events Page
  - https://www.nersc.gov/users/training/events/
- Training Past Events Page
  - Can choose "Filter by Year"
- NERSC YouTube Channel
  - https://youtube.com/c/NERSCTraining-HPC/
- Training Events Archive Page
- Training Materials Page
- Best Practices for NERSC Training Journal Paper, Slides

We welcome any suggestions, comments, ideas on Training!!

Coming up

Upcoming topics:

- Power/Energy Consumption @ NERSC
- Security @ NERSC
- Community needs/ideas (e.g. new groups/topics, "get to know" <blank>, new docs/training options, career?)
- Other topic suggestions/requests?

Lightning Talks

We'd love to hear more lightning talks **from NERSC users** about the research you use NERSC for!

Nominate a topic at: https://forms.gle/WjYx7zV7SAz2CaYz7

Science Highlights Submission:
https://docs.google.com/forms/d/e/1FAIpQLScP4bRCtcde43nqUx4Z_sz780G9HsXtpecQ_qIPKvGafDVVKQ/viewform

Highlights

HAPPY HOLIDAYS!

NeRSC

Thank You