Perlmutter Access, Allocations, & User Environment
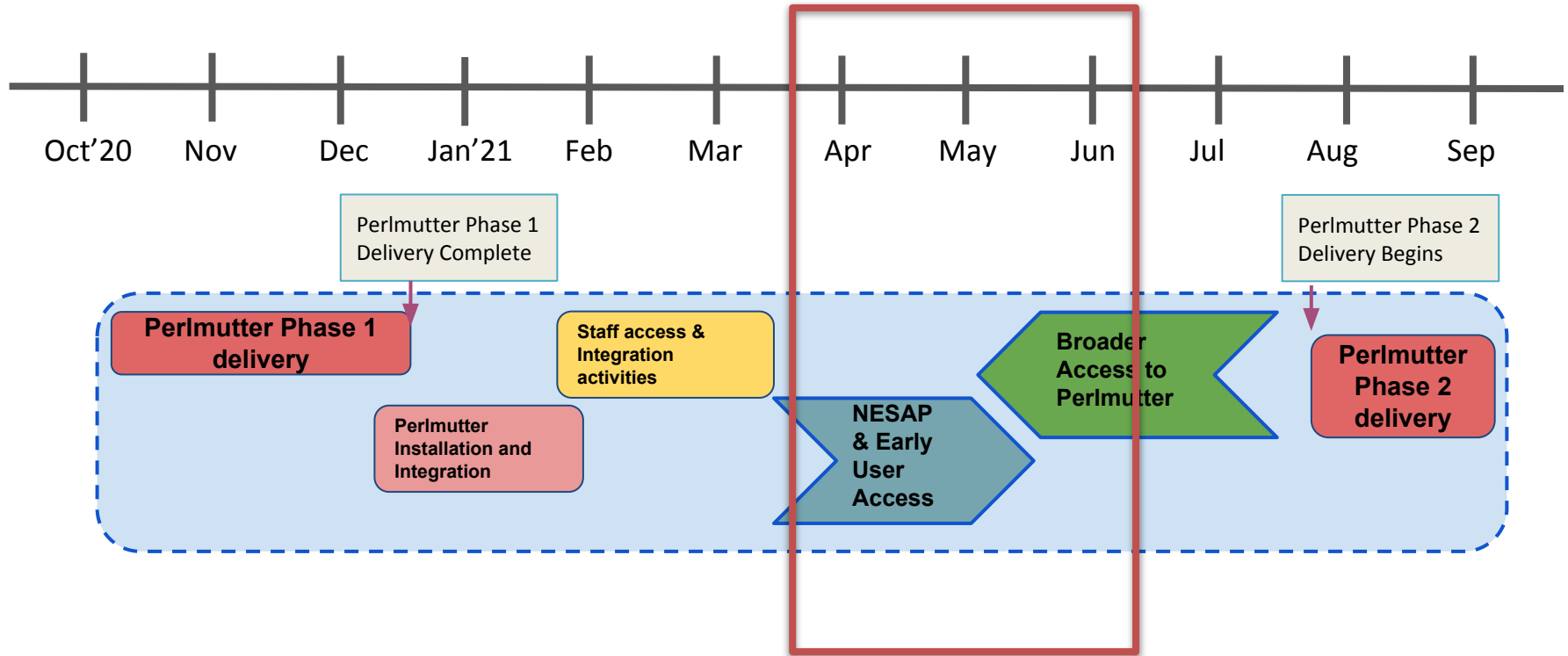
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2020 NERSC User Group
Annual Meeting

Rebecca Hartman-Baker
User Engagement Group Lead
August 17, 2020

Outline

- **Access & Allocations**
  - Timeline review
  - Access & Allocations
- **User Environment**
  - Conceptual Architecture
  - Logging in
  - Programming environment
  - Software
  - Running jobs
- **Learning Opportunities**
  - Training
  - Office Hours
  - Hackathons

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Perlmutter Phased Timeline

Oct'20 Nov Dec Jan'21 Feb Mar Apr May Jun Jul Aug Sep

Perlmutter Phase 1 Delivery Complete

Perlmutter Phase 2 Delivery Begins

Perlmutter Phase 1 delivery

Staff access & Integration activities

Perlmutter Installation and Integration

NESAP & Early User Access

Broader Access to Perlmutter

Perlmutter Phase 2 delivery

User Access to Perlmutter Phase I (GPU Nodes)

~ April 2021:

- All users given accounts to Phase I for code development and small-scale testing
- Priority access for large-scale testing and project milestones
  - NESAP teams
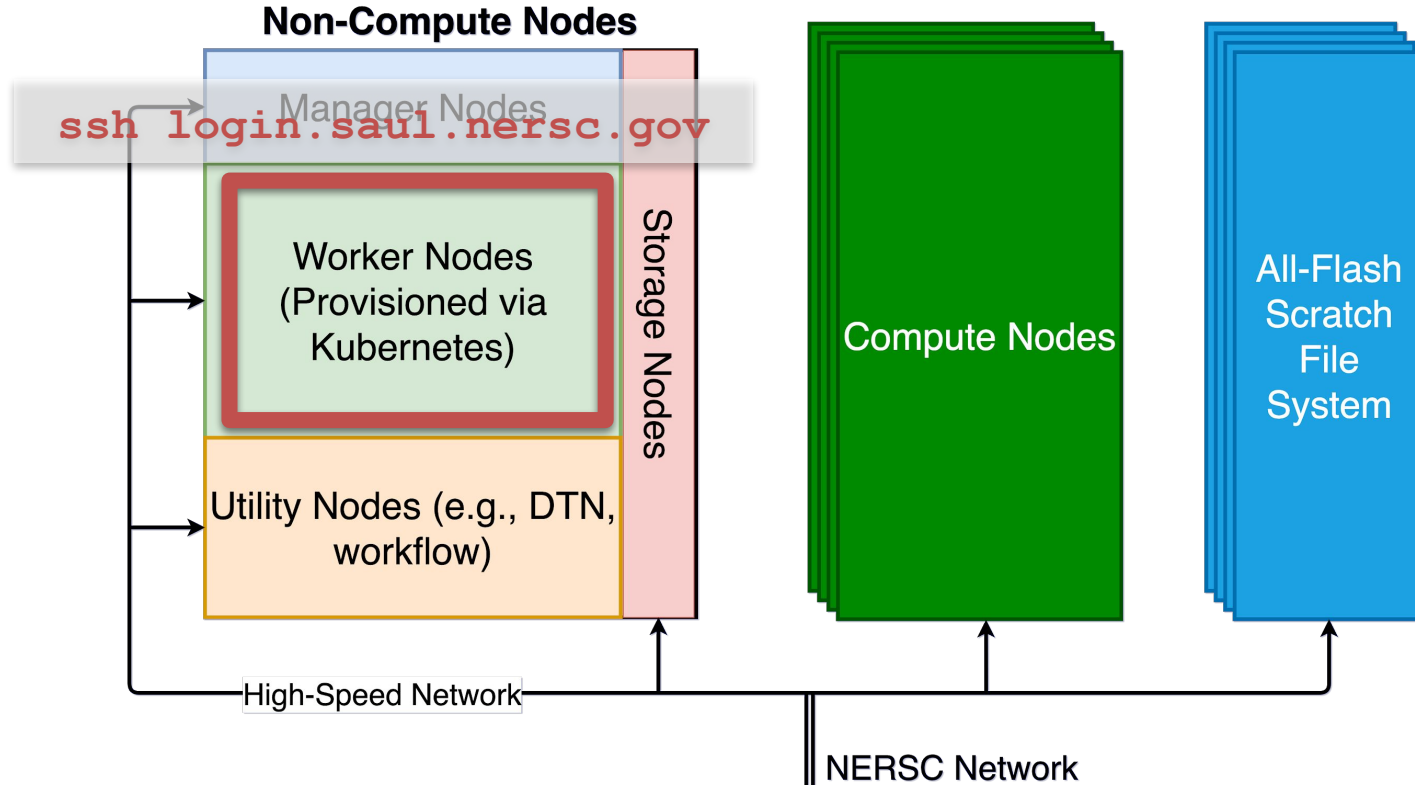 - Exascale Computing Project teams

~ May 2021:

- Large-scale scientific computing access for all GPU-capable projects
- GPU-readiness evaluation form required
- Key GPU-enabled community apps will be available

Allocations & Charging

- In Allocation Year (AY) 2021:
  - All time will be "free"
  - However, no commitment for hours available
  - *Expect that there will be outages for testing & stabilization*
- ERCAP requests & charging will begin in AY 2022
- Allocation and Charging Units
  - **GPU Node Hours** for Perlmutter GPU accelerated nodes
  - **CPU Node Hours** for Perlmutter CPU, Cori Haswell and KNL nodes
  - **GPU** & **CPU** hours will not be interchangeable!
  - CPU Node Hour charges will incorporate performance scale factors for 3 types of nodes

Perlmutter Architecture: Conceptual Overview

Non-Compute Nodes

Manager Nodes

`ssh login.saul.nersc.gov`

Worker Nodes (Provisioned via Kubernetes)

Utility Nodes (e.g., DTN, workflow)

Storage Nodes

Compute Nodes

All-Flash Scratch File System

High-Speed Network

NERSC Network

The Login Experience

- `ssh login.saul.nersc.gov`
- Each user within a container orchestrated by Kubernetes
  - Spin up resources as needed
  - Insulation from other users' behavior
- Jupyter also available for login

Login Node Environment

- Will be largely familiar to users
- Differences:
  - LMOD instead of modules (also on Cori in AY21*)
    - Hierarchical based modules, should be easier to find & load modules
  - Different programming environments
    - No Intel

*probably

Programming Environment

	GPU Support	Fortran/ C/C++	OpenACC 2.x	OpenMP 5.x	CUDA	Kokkos / Raja	Cray MPI
PGI	🟩	🟩	🟩	🟩	🟩	🟩	🟩
CCE		🟩				🟩	🟩
GNU	🟩	🟩	🟩	🟩	🟩	🟩	🟩
LLVM	🟦	🟦		🟦	🟦	🟦	🟦

Vendor Supported

NERSC Supported

Software

- NERSC and/or Vendor will provide many libraries for users
  - Available through LMOD modules (similar to current environment, with a few advantages)
- Users will be able to compile software not provided
  - User Spack instance, to draw upon pre-existing recipes
  - Help from NERSC consultants to install in user or project space
- New: Cray Minerva Data & Analytics Software Stack

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Software: Minerva Data & Analytics Stack

Library	Vendor Supported?	GPU Enabled?
Python (Anaconda)		
Spark		
R		
TensorFlow		
Keras		
Caffe		
PyTorch		

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Running Jobs

- Slurm will continue to be used for job scheduling
- Additional flag needed for requesting GPU resources
- Queue policies TBD, but should resemble Cori

Learning Opportunities: Training

- NERSC will hold training sessions for diverse interests and levels of experience
  - How to use the system
  - How to compile codes
  - Performance optimization
  - NVIDIA A100 Architecture deep dive
  - Development and tools
  - Machine Learning
  - Chemistry / materials science applications
  - and more!

Learning Opportunities: Office Hours

- Over past 2 years, we have developed & deployed office hours concept modeled after University office hours
  - Past topics included ERCAP, MFA, KNL
- We will continue to offer opportunities for one-on-one help with targeted topics
  - Replace open office hours with appointment scheduling
- We have some ideas for topics, but also will seek your feedback
  - Please look for survey in a few weeks

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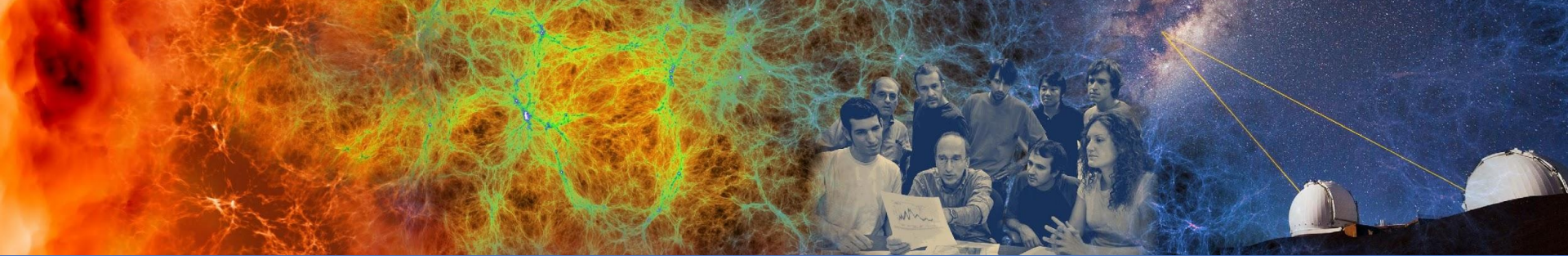
Learning Opportunities: Hackathons

- Hackathons come in a variety of forms, but generally:
  - Pair code teams with experienced mentors.
  - Give an opportunity learn new profiling techniques and tools.
  - Identify, explore and directly fix problems with your codes.
  - Research and learn about new coding strategies and methods.
  - Develop contacts for future collaboration, code development and support.
  - Virtual-only formats are being adopted, tested and expanded on now.

Types of Hackathons

	GPU Hackathons	Center of Excellence (COE) Hackathons	NERSC Hackathons
Host	NVIDIA, OpenACC organization & a local host.	NERSC / HPE	NERSC
Format	Intense, 4 day events with preparation & follow-up.	B.C.: 6 weeks of intense preparation with HPE/NVIDIA, 1 week of full-time hacking. Now: ~12 weeks of lower intensity work with HPE/NVIDIA Collaborative events	Variety of formats, but often 1-2 day events with speakers to start followed by hands-on with your code.
Frequency	Many events year round	Quarterly	periodically, thematic
More Info	https://www.gpuhackathons.org	See next slide!	NERSC Weekly Email & NERSC website

Upcoming COE Hackathons

- Seeking 4 NESAP teams to commit to ~12 weeks of collaboration with HPE/NVIDIA on GPU performance optimization/tuning of their codes
- All NESAP teams encouraged to apply
  - Teams who have already participated in hackathons are welcome to apply again
  - Tier 2 NESAP teams also encouraged to apply
- Please contact Brian Friesen <bfriesen@lbl.gov> if you are interested in participating

Any Questions?

Thank You!