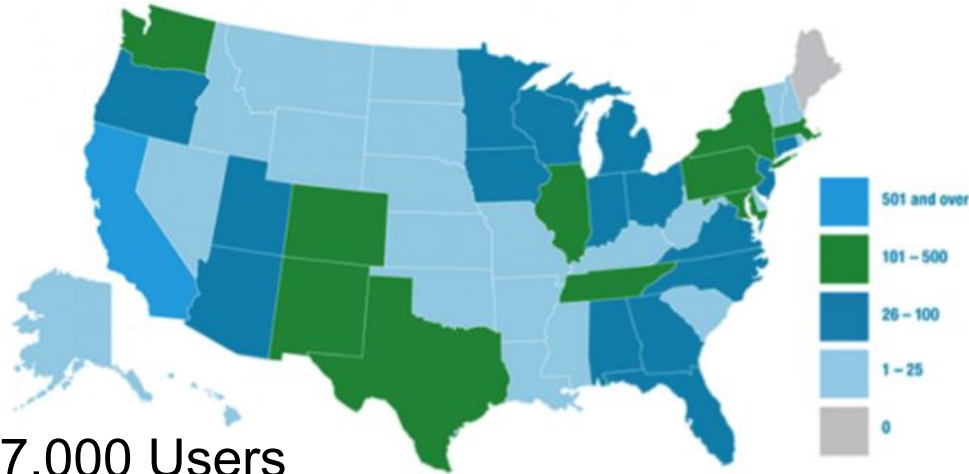# Programming for Perlmutter
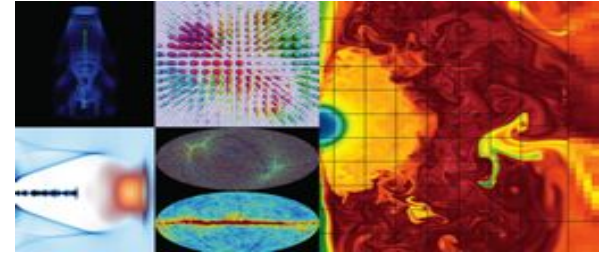
Jack Deslippe
NESAP Lead
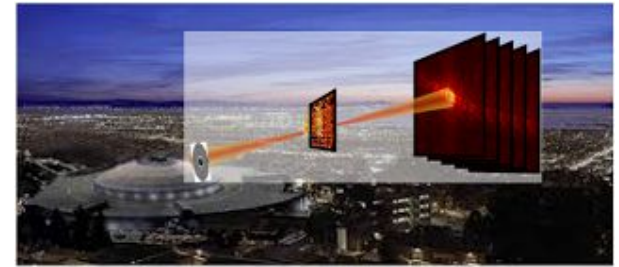Application Performance Group Lead

NERSC is the mission High Performance Computing facility for the DOE SC

7,000 Users
800 Projects
700 Codes
2000 NERSC citations per year

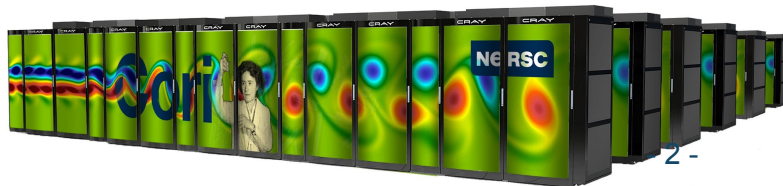
Simulations at scale

Data analysis support for DOE's experimental and observational facilities
Photo Credit: CAMERA

Lawrence Hall of Science

Advanced Light Source (ALS)

Berkeley Lab

Wang Hall
NERSC
ESnet

University of California, Berkeley

NERSC has a dual mission to advance science and the state-of-the-art in supercomputing

- We collaborate with computer companies years before a system's delivery to deploy advanced systems with new capabilities at large scale

- We provide a highly customized software and programming environment for science applications

- We are tightly coupled with the workflows of DOE's experimental and observational facilities – ingesting tens of terabytes of data each day

- Our staff provide advanced application and system performance expertise to users
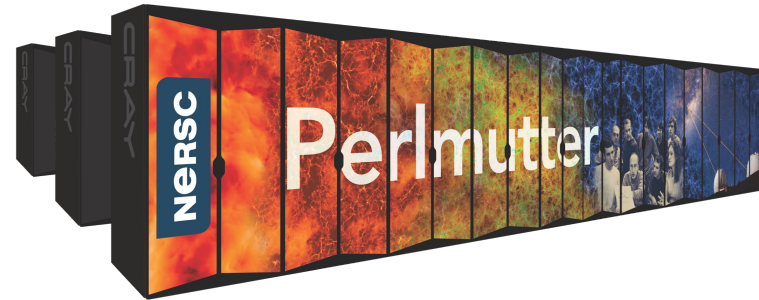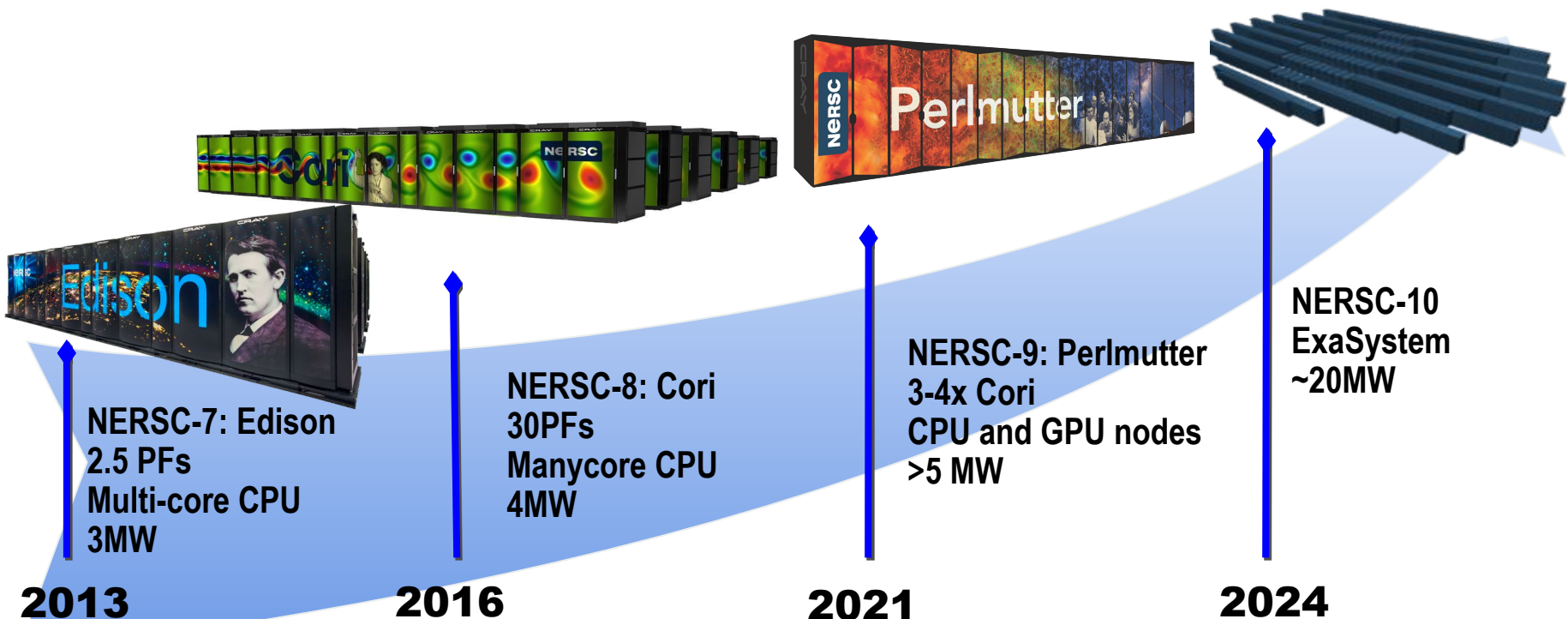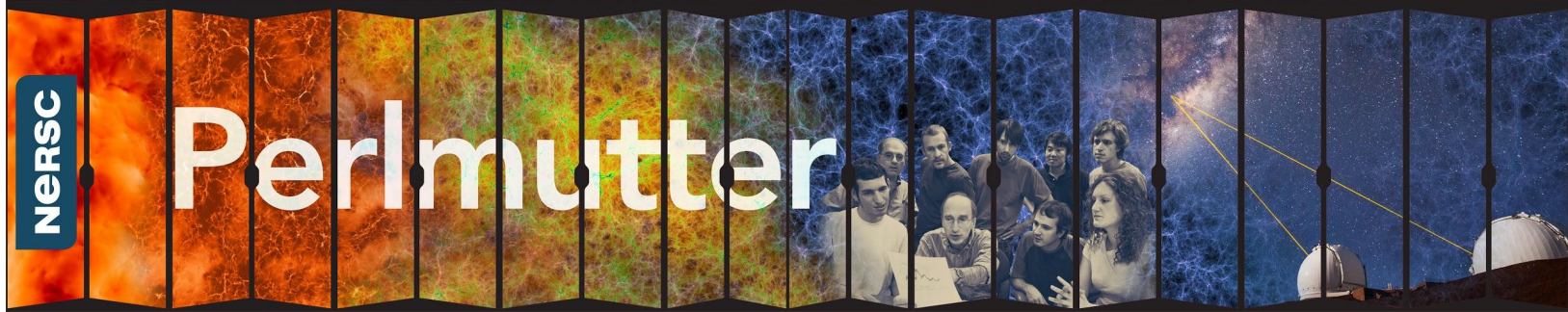
NERSC-9 will be named after Saul Perlmutter

- Winner of 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 to combine large scale simulations with experimental data analysis
- Login "saul.nersc.gov"

NERSC Systems Roadmap

2013

NERSC-7: Edison
2.5 PFs
Multi-core CPU
3MW

2016

NERSC-8: Cori
30PFs
Manycore CPU
4MW

2021

NERSC-9: Perlmutter
3-4x Cori
CPU and GPU nodes
>5 MW

2024

NERSC-10
ExaSystem
~20MW

- HPE Cray System with 3-4x capability of Cori

- GPU-accelerated (GPU/CPU) and CPU-only nodes

- HPE Cray Slingshot high-performance network

- All-Flash filesystem

- Application readiness program (NESAP)

Phase I: Arrived on February 22, 2021

- 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
- 35 PB FLASH scratch file system
- User access and system management nodes

Phase II Addition: Arrives This Fall

- 3,072 CPU only nodes
- 2 AMD "Milan" CPUs per node
- 512 GB memory per node
- Upgraded high speed network
- CPU partition will match or exceed performance of entire Cori system

Perlmutter Phase 1 Arrival
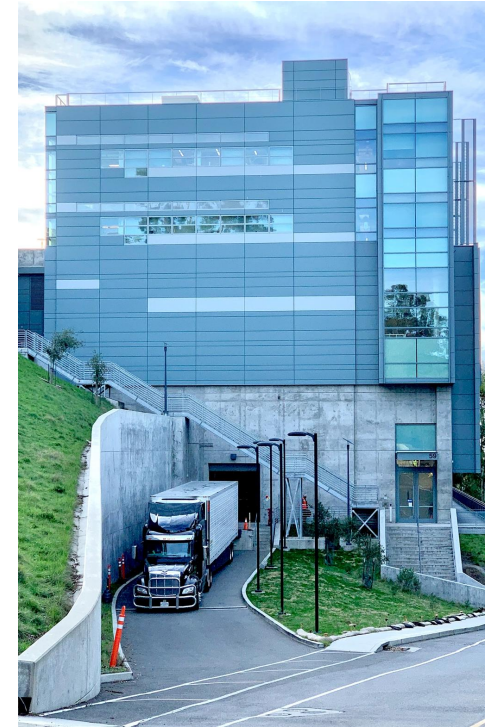
February 22, 2021

Perlmutter Programming Environments

	GPU Support	FORTRAN/C /C++	OpenACC 2.x	OpenMP 5.x	CUDA	Kokkos / Raja	Cray MPI
NVIDIA							
CCE							
GNU				(Community Effort)			
LLVM				(Community Effort)			

Vendor Supported

NERSC Supported

OpenMP NRE partnership with NVIDIA

- Agreed upon subset of OpenMP features to be included in the NVIDIA (was PGI) compiler

- OpenMP test suite created with micro-benchmarks, mini-apps, and the ECP SOLLVE V&V suite

- 5 NESAP application teams partnering with NVIDIA to add OpenMP target offload directives

- The production OpenMP offload compiler was released in April 2021.
  - Beta compiler was delivered in November 2020.
  - Offload capability was integrated into the NVIDIA HPC SDK compiler suite in December 2020.

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NERSC, NVIDIA to Partner on Compiler Development for Perlmutter System
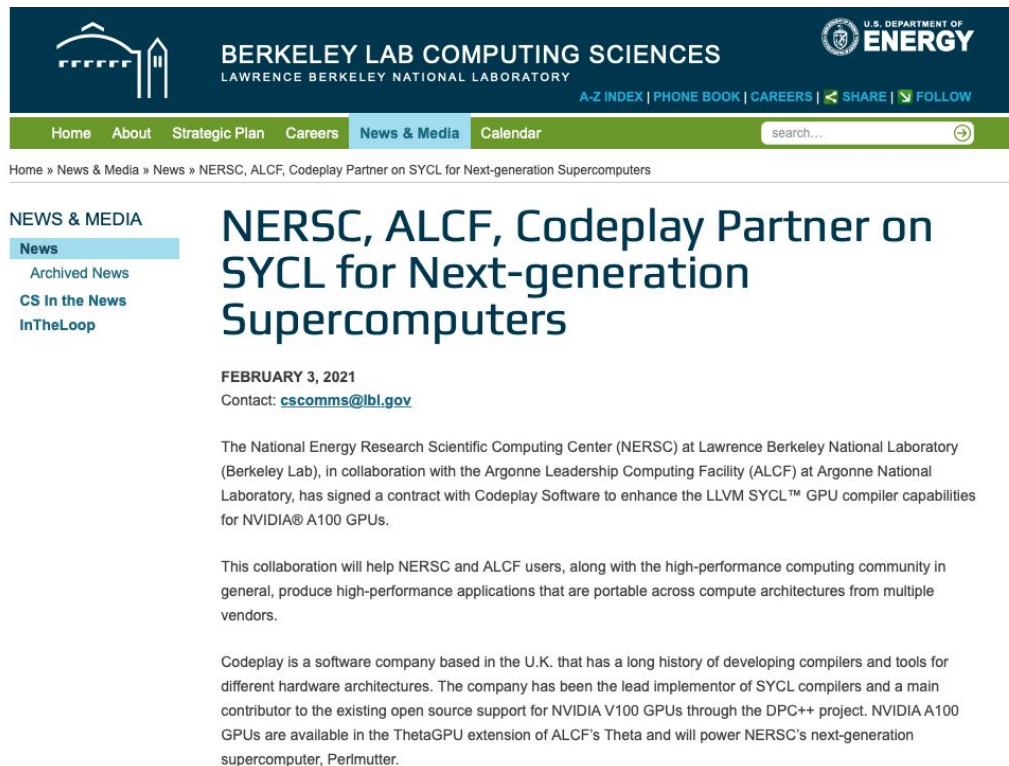
MARCH 21, 2019

The National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory (Berkeley Lab) has signed a contract with NVIDIA to enhance GPU compiler capabilities for Berkeley Lab's next-generation Perlmutter supercomputer.

In October 2018, the U.S. Department of Energy (DOE) announced that NERSC had signed a contract with Cray for a pre-exascale supercomputer named "Perlmutter," in honor of Berkeley Lab's Nobel Prize-winning astrophysicist Saul Perlmutter. The Cray Shasta machine, slated to be delivered in 2020, will be a heterogeneous system comprising both CPU-only and GPU-accelerated cabinets. It will include a new Cray system interconnect designed for data-centric computing; NVIDIA GPUs with new Tensor Core technology; CPU-only nodes based on next-generation AMD EPYC CPUs; direct liquid cooling; and an all-flash scratch filesystem that will move data at a rate of more than 4 terabytes/sec.

NERSC, ALCF and Codeplay partnership on SYCL

- Target SYCL 2020 (latest specification) support on Ampere A100 GPUs

- Open LLVM based compiler

- Provides Portability for Apps Developed for Aurora

- Extensions for A100
  - Asynchronous Copy
  - Asynchronous Barrier
  - Tensor core types/ APIs

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NERSC, ALCF, Codeplay Partner on SYCL for Next-generation Supercomputers

FEBRUARY 3, 2021
Contact: cscomms@lbl.gov

The National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory (Berkeley Lab), in collaboration with the Argonne Leadership Computing Facility (ALCF) at Argonne National Laboratory, has signed a contract with Codeplay Software to enhance the LLVM SYCL™ GPU compiler capabilities for NVIDIA® A100 GPUs.

This collaboration will help NERSC and ALCF users, along with the high-performance computing community in general, produce high-performance applications that are portable across compute architectures from multiple vendors.

Codeplay is a software company based in the U.K. that has a long history of developing compilers and tools for different hardware architectures. The company has been the lead implementor of SYCL compilers and a main contributor to the existing open source support for NVIDIA V100 GPUs through the DPC++ project. NVIDIA A100 GPUs are available in the ThetaGPU extension of ALCF's Theta and will power NERSC's next-generation supercomputer, Perlmutter.

Many NERSC Applications Actively Working w/ OpenMP Offload

- BerkeleyGW
- Quantum ESPRESSO
- WEST
- GAMESS
- QMCPACK
- LAMMPS
- US QCD Apps
- Kokkos Apps w/ OpenMP Back-end