

# Computing Sciences at Berkeley Lab

CS Student Program Welcome

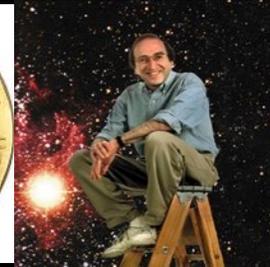
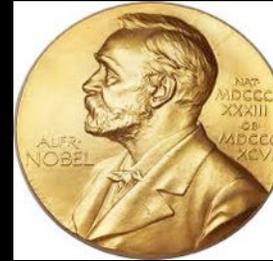
2 June 2020

**David Brown, Director**  
**Computational Research Division**  
**Lawrence Berkeley National Laboratory**



# Why the nation needs national laboratories

- Discovery science
- Scientific solutions addressing national challenges, especially energy
- Unique scientific capabilities
  - User facilities
- Managed, large research teams
- Important technologies with long, risky R&D paths
- A diverse group of highly trained, creative, and committed scientists and engineers.



# Berkeley Lab is one of the 17 U.S. Department of Energy (DOE) National Laboratories

## Office of Science Laboratories

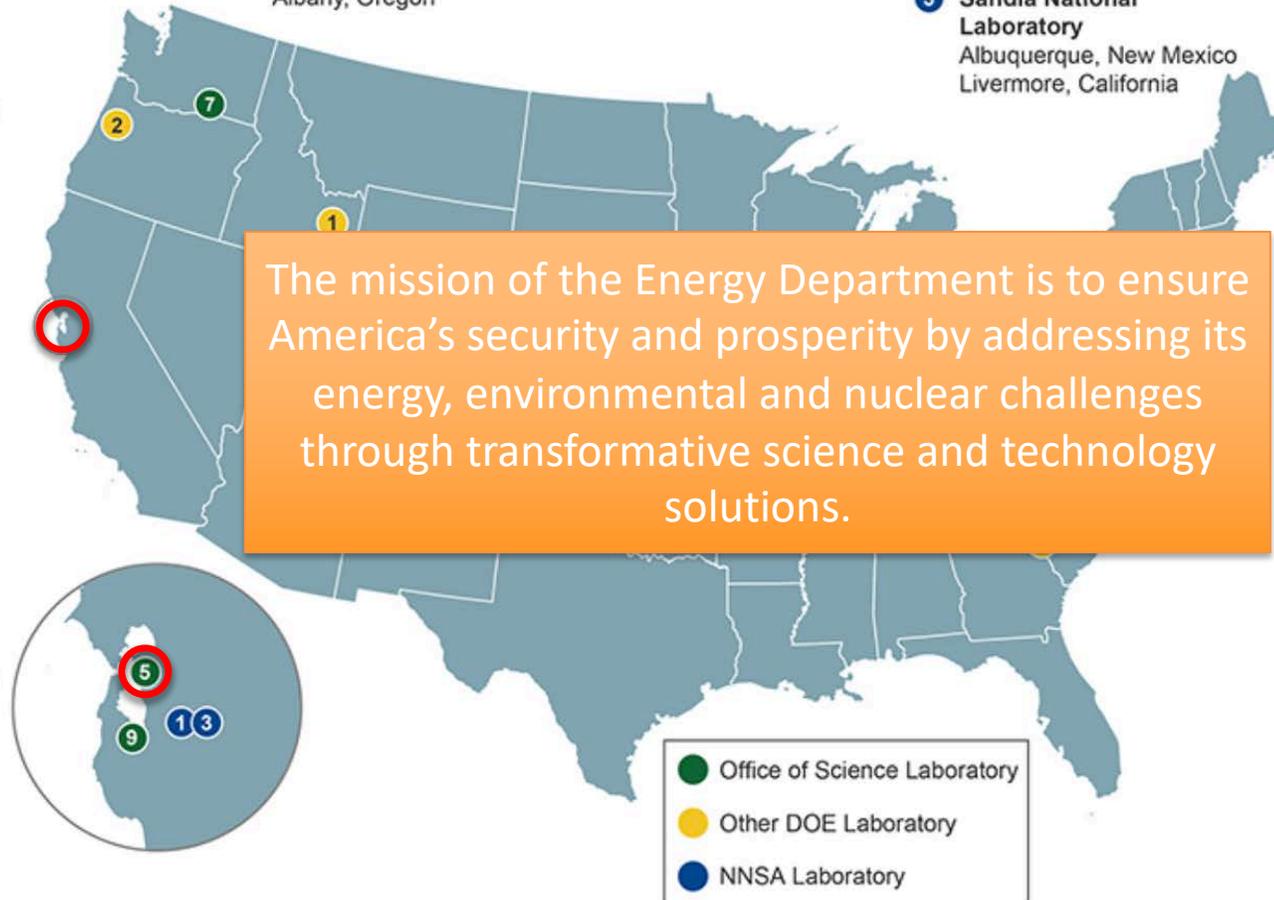
- 1 Ames Laboratory  
Ames, Iowa
- 2 Argonne National Laboratory  
Argonne, Illinois
- 3 Brookhaven National Laboratory  
Upton, New York
- 4 Fermi National Accelerator Laboratory  
Batavia, Illinois
- 5 Lawrence Berkeley National Laboratory  
Berkeley, California
- 6 Oak Ridge National Laboratory  
Oak Ridge, Tennessee
- 7 Pacific Northwest National Laboratory  
Richland, Washington
- 8 Princeton Plasma Physics Laboratory  
Princeton, New Jersey
- 9 SLAC National Accelerator Laboratory  
Menlo Park, California
- 10 Thomas Jefferson National Accelerator Facility  
Newport News, Virginia

## Other DOE Laboratories

- 1 Idaho National Laboratory  
Idaho Falls, Idaho
- 2 National Energy Technology Laboratory  
Morgantown, West Virginia  
Pittsburgh, Pennsylvania  
Albany, Oregon
- 3 National Renewable Energy Laboratory  
Golden, Colorado
- 4 Savannah River National Laboratory  
Aiken, South Carolina

## NNSA Laboratories

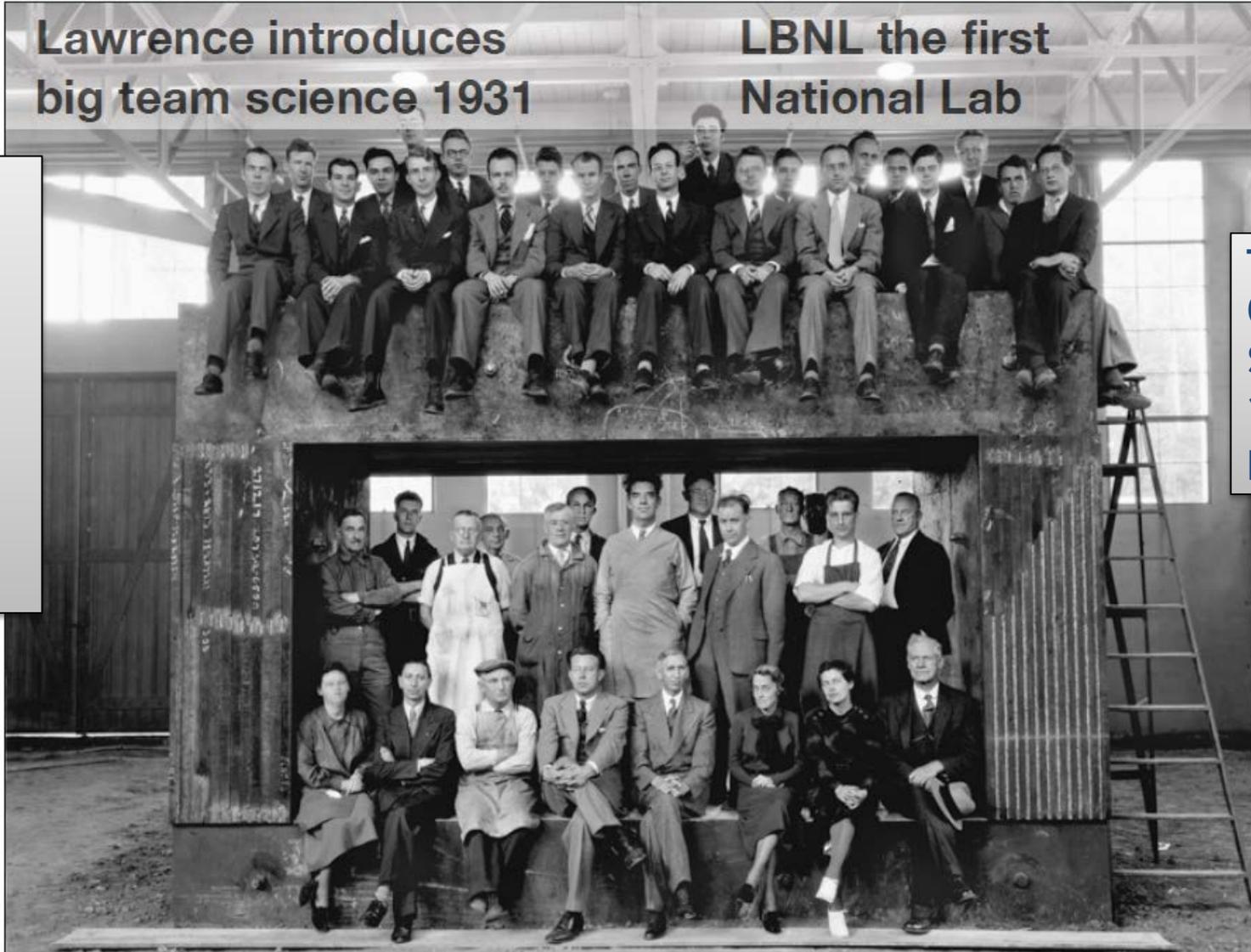
- 1 Lawrence Livermore National Laboratory  
Livermore, California
- 2 Los Alamos National Laboratory  
Los Alamos, New Mexico
- 3 Sandia National Laboratory  
Albuquerque, New Mexico  
Livermore, California



# Berkeley Lab Changes Science

Lawrence introduces  
big team science 1931

LBL the first  
National Lab

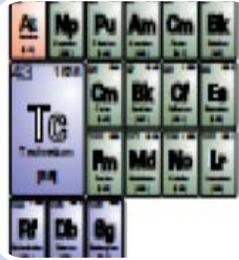


Radiation Lab staff on the  
magnet yoke for the 60-inch  
cyclotron, 1939, including:

E. O. Lawrence  
Edwin McMillan  
Glenn Seaborg  
Luis Alvarez  
J. Robert Oppenheimer  
Robert R. Wilson

Today, Berkeley Lab has:  
Over 4000 employees  
\$1.1B in FY18 funding  
13 associated Nobel  
prizes

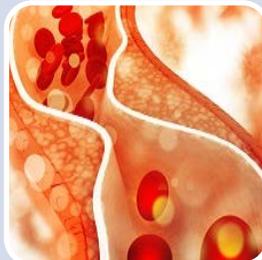
# Berkeley Lab brings Science Solutions to the World



Discovered 16 elements



Unmasked a dinosaur killer



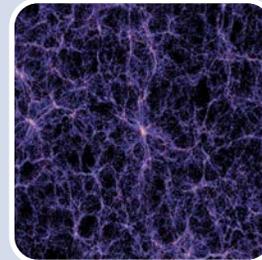
Identified good and bad cholesterol



Fabricated the smallest machines



Turned windows into energy savers



Confirmed the Big Bang and discovered dark energy



Explained Photosynthesis



Revealed the secrets of the human genome



<https://www.lbl.gov/program/35-breakthroughs/>



Molecular Foundry

ALS-Advanced Light Source

Bldg 50

Wang Hall  
Bldg 59

# Computing Sciences at Berkeley Lab in 2020



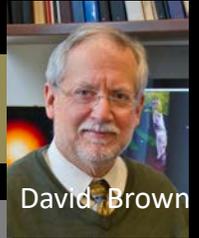
Jonathan Carter

## NERSC



Sudip Dosanjh

## Computational Research



David Brown



## Computational Science

## Applied Mathematics

$$\begin{aligned} \frac{dVar(t)}{dt} &= \\ &= -K^2 Fg + gK^2 F ds - \int_{s(t)}^{s(t)+S} (-g^{-1} F_s)_s - K \\ &= - \int_{s(t)}^{s(t)} (g^{-1} F_s)_s ds + \int_{s(t)}^{s(t)+S} (g^{-1} F_s)_s ds \\ &= [g^{-1} F_s |_{s(t)} - g^{-1} F_s |_{s(t)}] + [g^{-1} F_s |_{s(t)+S} - g^{-1} F_s |_{s(t)}] \\ &= -2 (g^{-1} F_s K_s) |_{s(t)} + 2 (g^{-1} F_s K_s) |_{s(t)} \end{aligned}$$

## Scientific Networking: ESnet

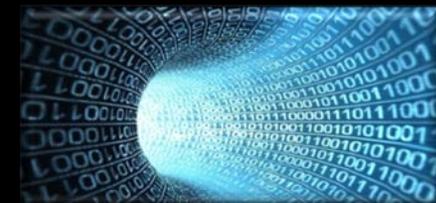


Inder Monga



## Computer Science

## Data Science & Technology



# NERSC at Berkeley Lab Provides HPC and Data Resources for Science Research



U.S. DEPARTMENT OF ENERGY

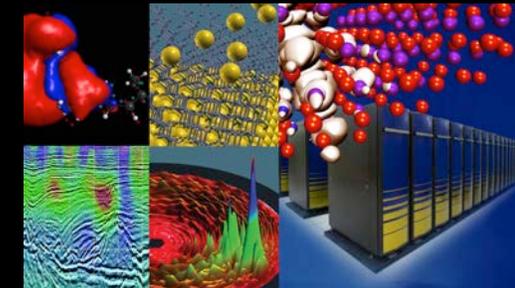
Office of

Largest funder of physical science research in U.S.

## NOW COMPUTING

A small sample of massively parallel scientific computing jobs running right now at NERSC.

PROJECT	MACHINE	NODES	NERSC HOURS USED
<b>Guest-host interactions in the gas phase, in aqueous systems and hydrate lattices: Implications for H2 storage and CO2 sequestration</b> PI: Sotiris Xantheas, Pacific Northwest National Laboratory (PNNL)	Cori	1,024	638,817.1



Materials, Chemistry,

Computing PI: Salma	Jun 11 11 AM - 12 PM	<a href="#">NERSC: Scientific Discovery through Computation</a>	<a href="#">Rebecca Hartman-Baker</a> (NERSC)	zoom
partnersh simulation PI: Choor Laboratory	Jun 11 1 PM - 3 PM	<a href="#">Introduction to NERSC Resources</a>	<a href="#">Helen He</a> (NERSC)	zoom
Computing PI: Salma	Jun 17 10 AM - 12	<a href="#">Crash Course in Supercomputing</a>	<a href="#">Rebecca Hartman-Baker</a> (NERSC)	zoom

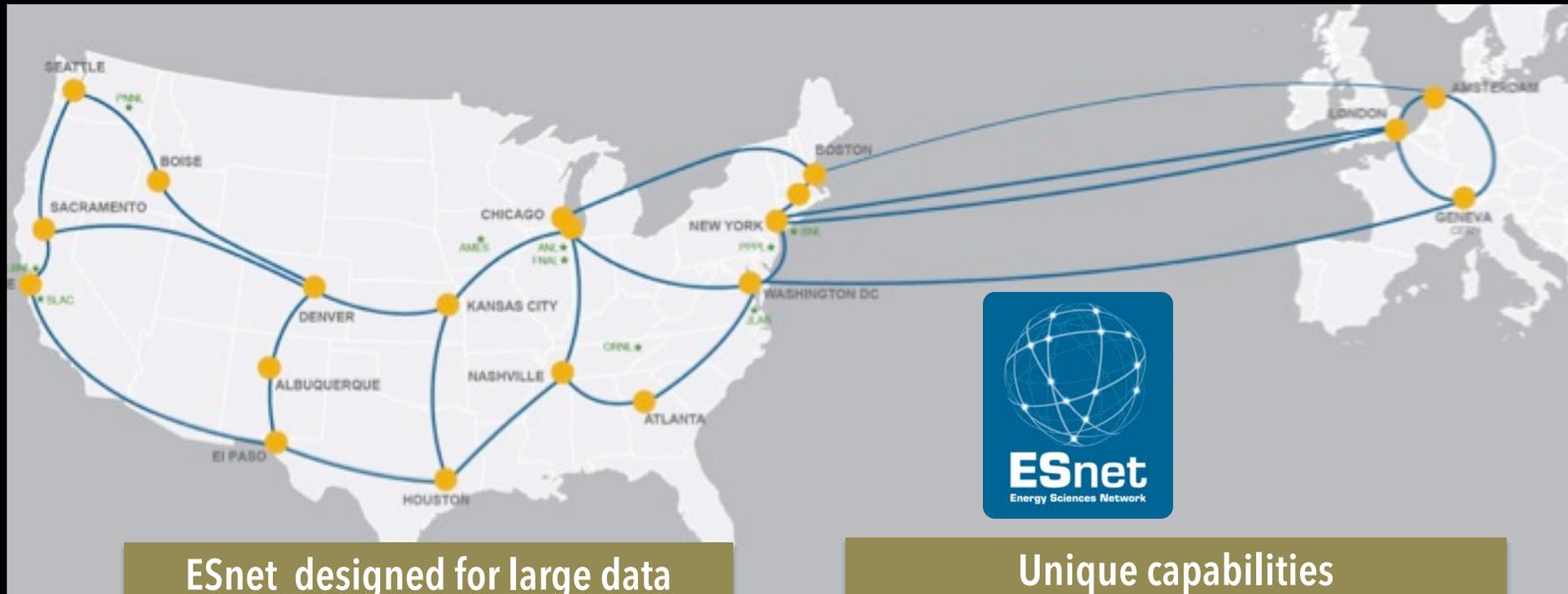
# National Energy Research Scientific Computing Center

# NERSC's newest machine Cori supports both the HPC Workload and Data-Intensive Science

- **Cray system with 9,300 Intel Knights Landing compute nodes**
  - Self-hosted, (not an accelerator) manycore processor  $> 64$  cores per node
  - On-package high-bandwidth memory at  $>400\text{GB/sec}$
- **Data Intensive Science Support**
  - 10 Haswell processor cabinets (Phase 1) to support data intensive applications
  - NVRAM Burst Buffer with 1.5PB of disk and 1.5TB/sec
  - 28 PB of disk,  $>700\text{ GB/sec}$  I/O bandwidth in Lustre bandwidth



# ESnet is a Unique Instrument for Science



## ESnet designed for large data

- Connects 40 DOE sites to 140 other networks
- Growing twice as fast as commercial

## Unique capabilities

- First 100G continental scale network
- ANI dark fiber can be leveraged to develop and deliver 1 terabit

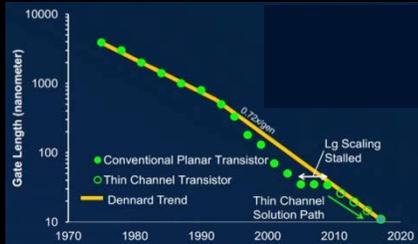
Jul 23  
11 AM - 12  
PM

[From Simulations to Real-World: Building Deep Reinforcement Learning for Networks](#)

[Mariam Kiran](#) (Scientific Data Management Group)

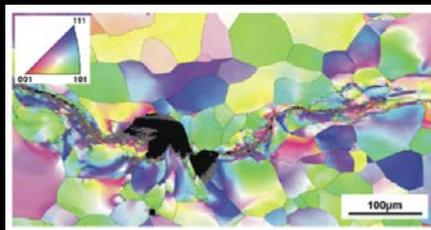
zoom

# What are the questions driving research in computing?



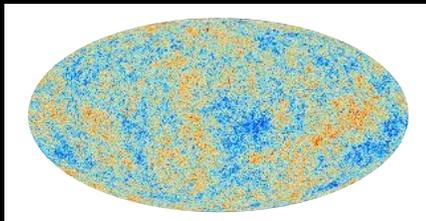
Limits of Chip Technology

Can we continue the growth in computing performance through more efficient architectures or new paradigms?



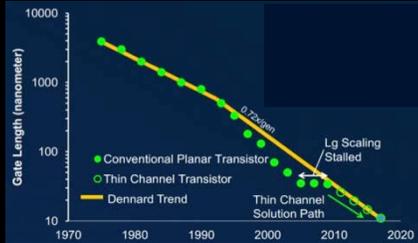
Interfaces Key at Mesoscale

What mathematical models, algorithms and software are needed for increasingly complex scientific theories and experimental data sets?



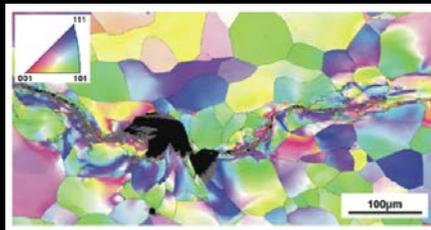
Can we enable new modes of scientific discovery by applying advanced computing and networking to data from science experiments?

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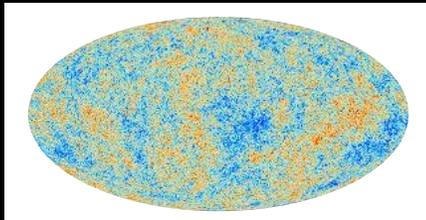
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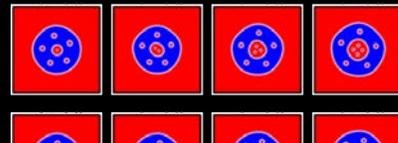
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# Future of computing: Extreme Heterogeneity? Quantum?

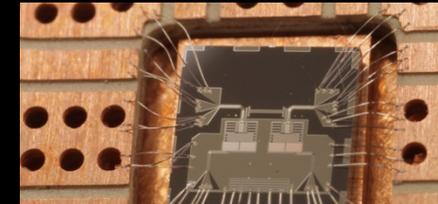
Can new logic devices give us beyond-Moore performance?

Quantum Simulation for Materials, Chemistry and Physics

Investigating alternative devices



Multiple quantum device



Use Skirm act as info for multi-v

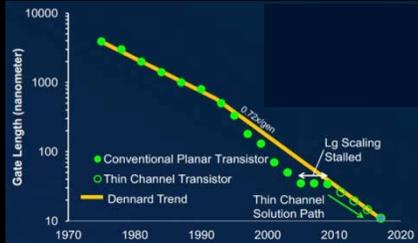
Investigat architectu magnetic Flux Quan

Jun 16 11 AM - 12 PM	<a href="#">Unitary Matrix Decompositions for Quantum Circuit Synthesis</a>	<a href="#">Roel Van Beeumen</a> (Scalable Solvers Group)	zoom
Jul 07 11 AM - 12 PM	<a href="#">Challenges in Building Quantum Computers</a>	<a href="#">Anastasiia Butko</a> (Computer Architecture Group)	zoom
Jul 14 11 AM - 12 PM	<a href="#">Ultrascale System Interconnects at the end of Moore's Law</a>	<a href="#">John Shalf</a> (Computer Science Department)	zoom



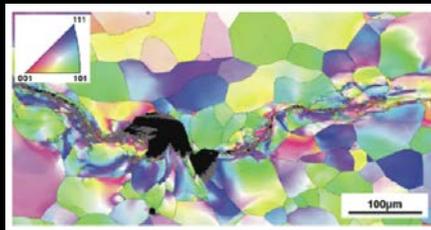
THE HAMILTONIAN LANDSCAPE FOR QUANTUM SIMULATION

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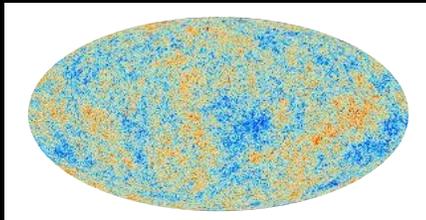
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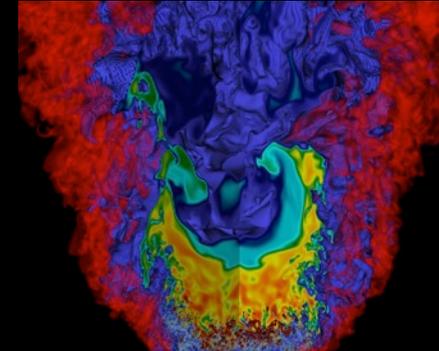


Can we enable new modes of scientific discovery by applying advanced computing and networking to data from science experiments?

## Transforming how we compute:

"smart" math, numerics, HPC: gives unprecedented capability

- **Smart math leads to science not possible before**
  - Use mathematical properties to build better simulation models
  - Simulation at previously inaccessible scales
  - Exploit matrix structure for faster linear algebra

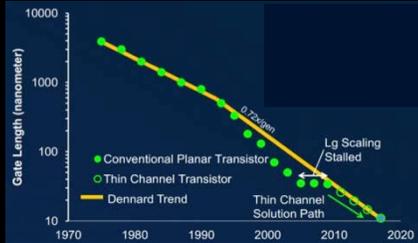


Jun 04 11 AM - 12 PM	<a href="#">Modeling Antarctic Ice with Adaptive Mesh Refinement</a>	<a href="#">Dan Martin</a> (Applied Numerical Algorithms Group)	zoom
Jun 25 11 AM - 12 PM	<a href="#">Surrogate Optimization for HPC Applications</a>	<a href="#">Juliane Mueller</a> (Center for Computational Sciences and Engineering)	zoom
Jul 09 11 AM - 12 PM	<a href="#">Simulating Supernovae with Supercomputers</a>	<a href="#">Donald Willcox</a> (Center for Computational Sciences and Engineering)	zoom

Over 100x increase in throughput

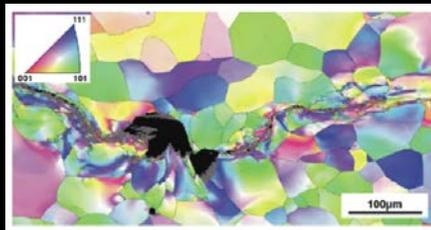
MAESTRO simulation near ignition showing flow from center of star and region of high energy generation

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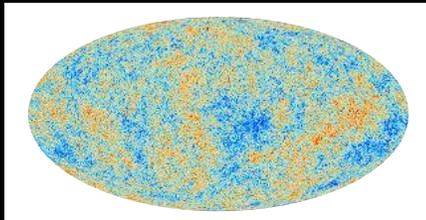
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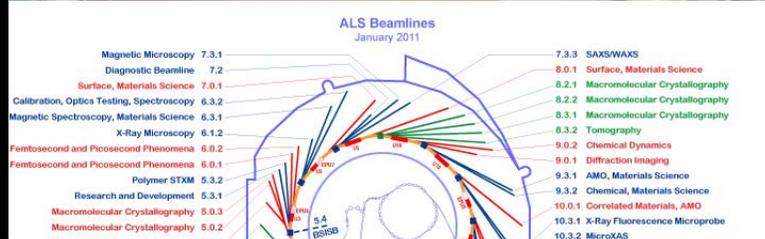
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# The Advanced Light Source (ALS) hosts dozens of different experiments and end station detectors



Jul 28  
11 AM - 12  
PM

[Towards a BES Light Source Wide Event-triggered Tomography Data Analysis Pipeline Using a Sustainable Software Stack](#)

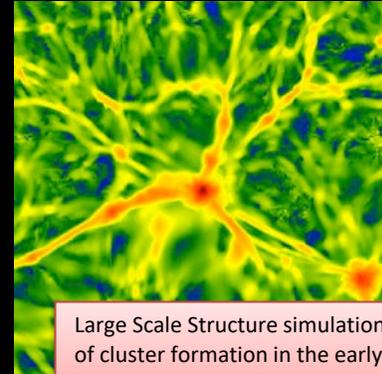
[Hari Krishnan](#) (Data Analytics and Visualization Group)

zoom



# Data-driven scientific discovery requires integration of modeling, simulation, analysis, data management

- **Example: 21<sup>st</sup> Century Cosmology:**
  - Tight collaboration between astrophysicists and computational scientists to develop new technologies for cosmological data



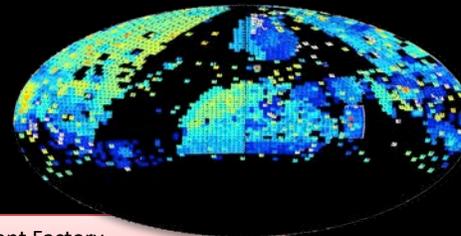
Large Scale Structure simulations of cluster formation in the early



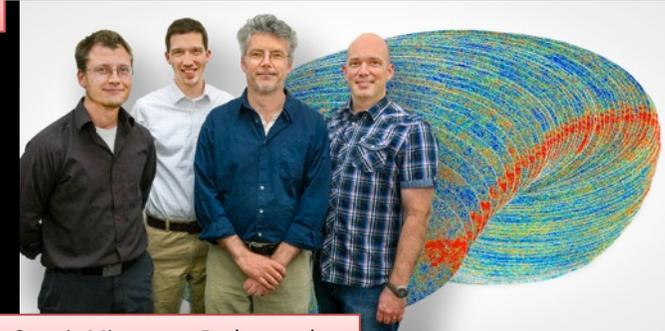
Jun 18 11 AM - 12 PM	<a href="#">High Performance Computing For Cosmic Microwave Background Data Analysis</a>	<a href="#">Julian Borrill</a> (Computational Cosmology Center)	zoom
Jun 30 11 AM - 12 PM	<a href="#">Efficient Scientific Data Management on Supercomputers</a>	<a href="#">Suren Byna</a> (Scientific Data Management Group)	zoom

modeling & simulation of supernovae and large-scale structure formation

explosion

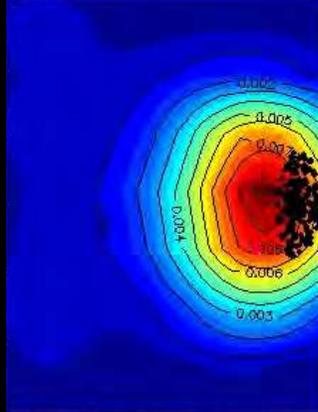


Palomar Transient Factory data-analysis sky-coverage map for the first 3 years of the project



Cosmic Microwave Background Radiation data from Planck

# Machine Learning enables new scientific discoveries from massive data sets



Identifying particle

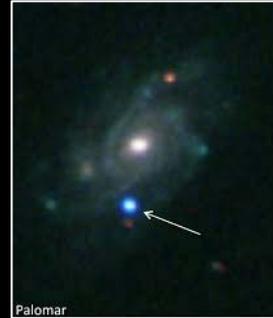
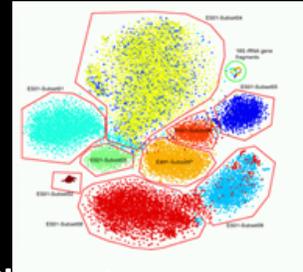
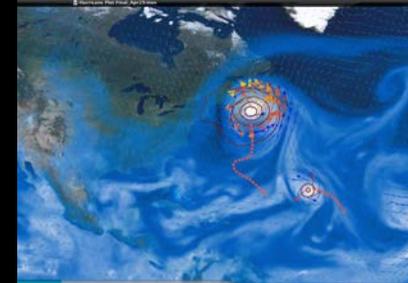


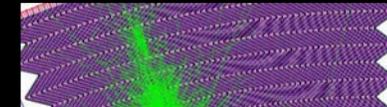
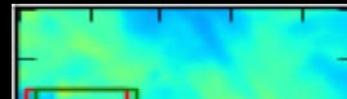
Image analysis in cosmology and light sources



Clustering genes and finding networks



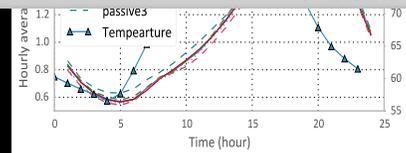
Identifying hurricanes



Jun 23 11 AM - 12 PM	<a href="#">Rise of the Machines</a>	<a href="#">Prabhat</a> (NERSC)	zoom
Jul 02 11 AM - 12 PM	<a href="#">Neural Networks with Euclidean Symmetry for Physical Sciences</a>	<a href="#">Tess Smidt</a> (Computational Chemistry, Materials & Climate Group)	zoom

Brain 3D model reconstruction

Decision support for energy infrastructure



Modeling human behavior

- Projects that advance the state-of-art in machine learning with ties to science



**Welcome to Berkeley Lab Computing Sciences!**