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Oppenheimer Science and Energy Leadership Program (OSELP)

Simulation and Computation at LANL

Speaker

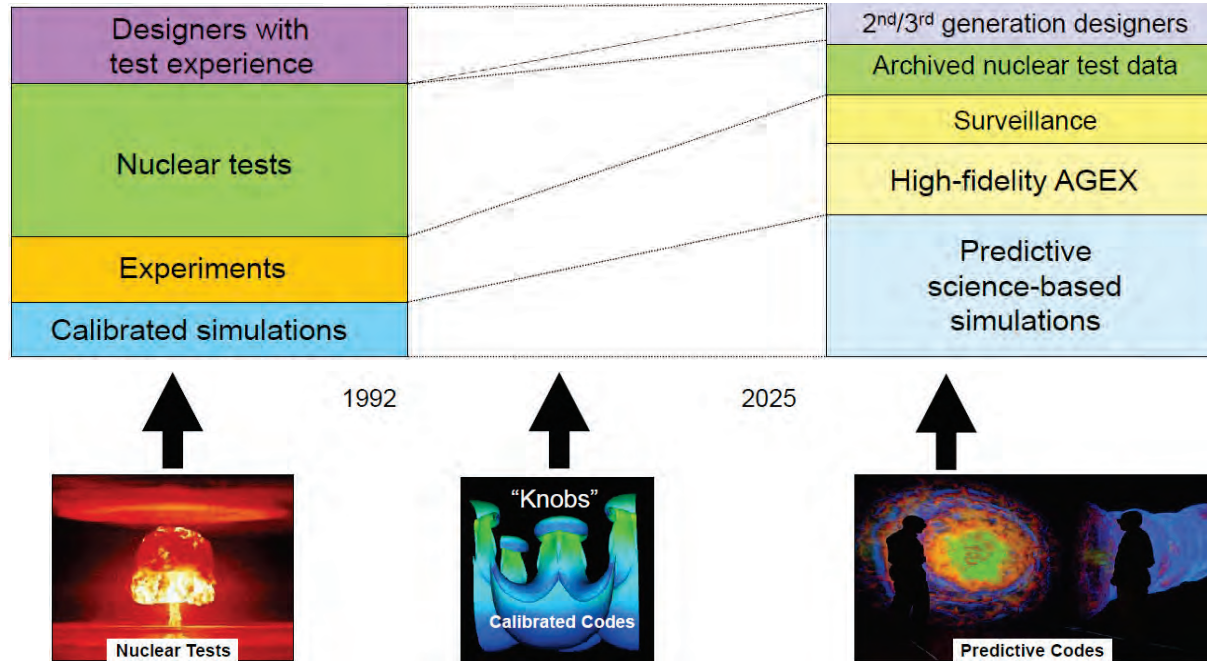
Irene Qualters/ALDSC

March 7, 2022

Additional Panel Members

- **Jim Lujan**, Project-Program Director
 - Programs: ASC (Crossroads, CTS-2), Multiprogram Institutional Computing Platforms (Venado)
- **Mark Schraad**, Division Leader of Computational Physics, Weapons Directorate
 - Research in Computational Physics and the development of codes, models, algorithms, IS&T Advisory Council
 - Programs: ASC, Science, LDRD (Lab-directed Research & Development)
- **Aric Hagberg**, Deputy Division Leader of Computer, Computational and Statistical Sciences, STE Directorate
 - Programs: ASC, Science, LDRD
 - Leading development of LANL's AI vision, strategy and plan, IS&T Leadership Team

Simulation and Computation plays a pivotal role in maintaining confidence in the stockpile as the approach to underwrite that confidence has changed



*The need for resolution and fidelity at scale
drives our need for increased computing capability*

DOE/NNSA Advanced Simulation and Computing (ASC) program provides the computational surrogate for testing

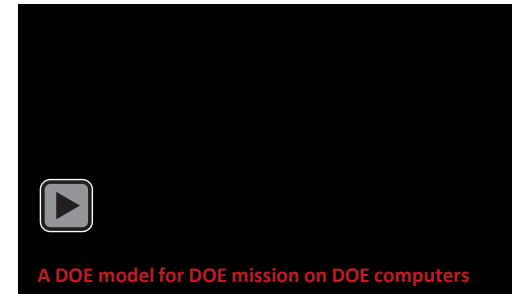
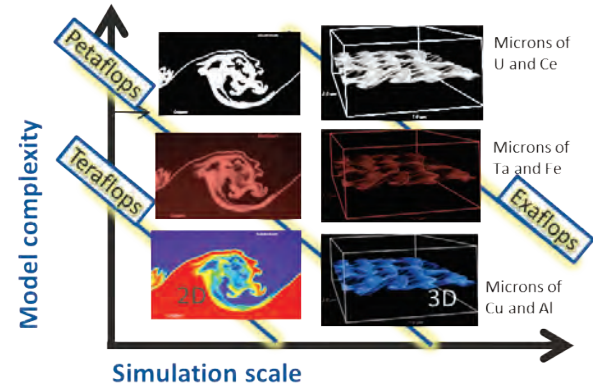
“Under ASC, computer simulation capabilities are developed to analyze and predict the performance, safety, and reliability of nuclear weapons and to certify their functionality.”



ASC provides simulation-based confidence in the U.S. stockpile

New advances in predictive multiscale modeling, simulation, and computation are required to address both urgent and longer-term NNSA needs

- **Urgent national security drivers: Stockpile aging has brought a steady drumbeat of complex and unexpected challenges**
 - Components deteriorate in operational environments
 - Materials change with intrinsic radiation
 - Material properties may change over time
- **Among longer-term national security issues requiring higher resolution:**
 - Nuclear device disablement
 - 3D assessment of surety options
 - Understanding plutonium
 - Determining the effects of hydrodynamic mixing on performance
- **Similar challenges and motivations exist in many science fields**
 - e.g., seismic, astrophysics, pandemic prediction & response....



**Our capability pillars
define six key areas of
science, technology,
and engineering in
which we must lead**

MATERIALS FOR THE FUTURE	Defects and Interfaces Extreme Environments Emergent Phenomena
NUCLEAR AND PARTICLE FUTURES	Accelerator Science & Technology Applied Nuclear Science & Engineering High Energy Density Plasmas & Fluids Nuclear, Particle, Astrophysics & Cosmology
INTEGRATING INFORMATION, SCIENCE, AND TECHNOLOGY FOR PREDICTION	Computing Platforms Computational Science Data Science
SCIENCE OF SIGNATURES	Nuclear Detonation Nuclear Processing, Movement, Weaponization Natural and Anthropogenic Phenomena
COMPLEX NATURAL AND ENGINEERED SYSTEMS	Human–Natural System Interactions: Nuclear Engineered Systems Human–Natural System Interactions: Non-Nuclear
WEAPONS SYSTEMS	Design Manufacturing Analysis

Integrating Information, Science and Technology for Prediction *is a foundational pillar, informing and informed by all pillars*

Three themes

Computing Platforms

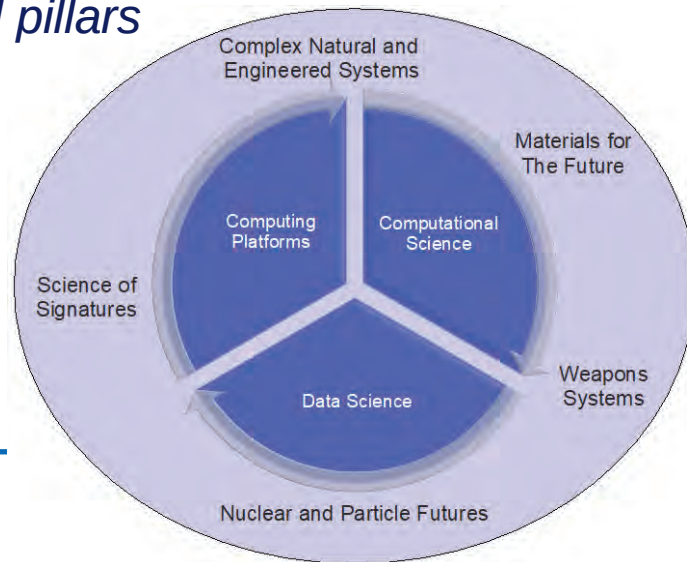
Architecture, Technologies, and Infrastructure

Computational Science

Methods, Algorithms, and Implementations to Advance Prediction

Data science

Analytics, Management, Sharing, Integrity



Four decadal goals

Quantum Computing

Realize quantum advantage for mission-relevant challenges in science and security

Transform Simulation

Revitalize high fidelity multi-physics, multi-scale simulation for prediction, control, and decision-making

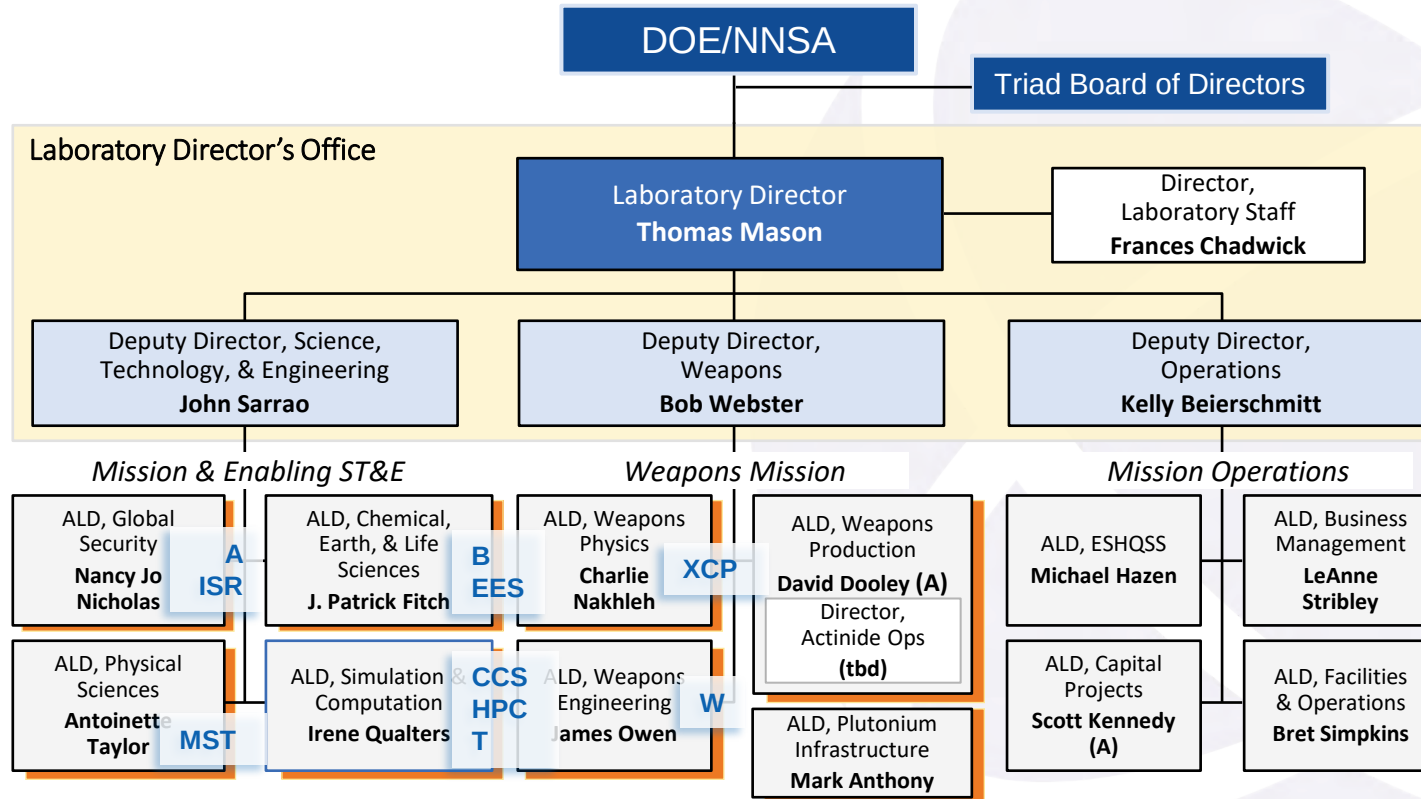
Data for Scientific Insight

Advance proficiency in data science for diverse and dynamic data, growing excellence in science and security programs

Information Integrity

Respond to emerging integrity challenges due to volume, security, and complexity of data, software, and workflow

IS&T capabilities span LANL organizational structure



Divisions with >25% efforts in IS&T

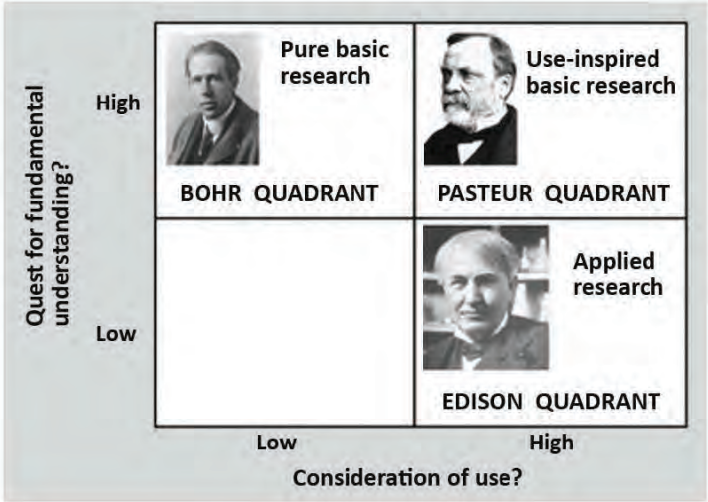
LANL IS&T is rooted in principles of CoDesign and Use-Inspired Research

Integrated, cross-disciplinary, mission-driven, encompassing evolution and revolution



Co-design ... it's in our DNA

Theory, Model

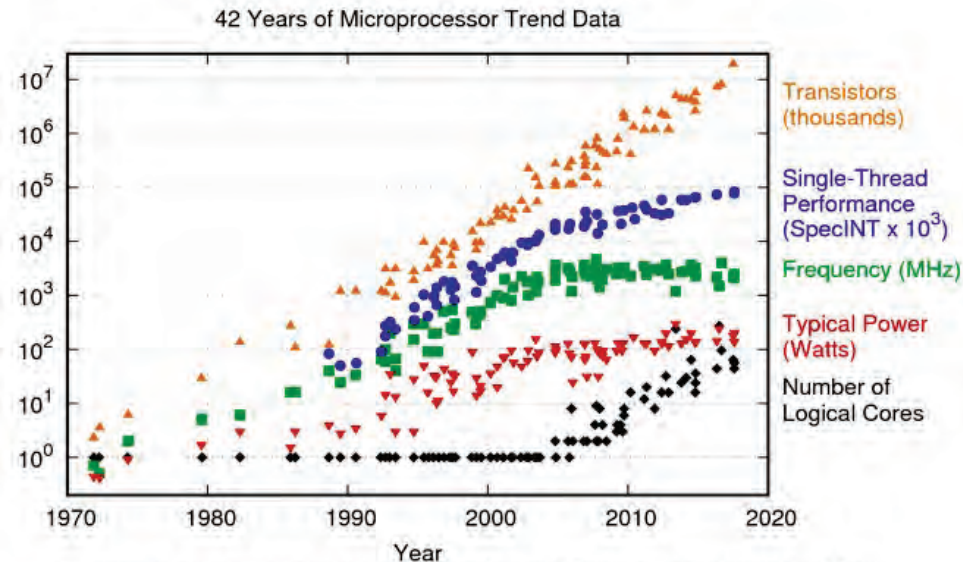


Accelerating Discovery,
Prediction, Design

High Performance
Computing,
Simulation,
Analysis

Experiment,
Observational
Data

After decades, the increasing benefits of “Moore’s law” and Dennard’s scaling, essential to meeting computational performance demands, have gradually stalled



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and G. Batten
New plot and data collected for 2010-2017 by K. Rupp

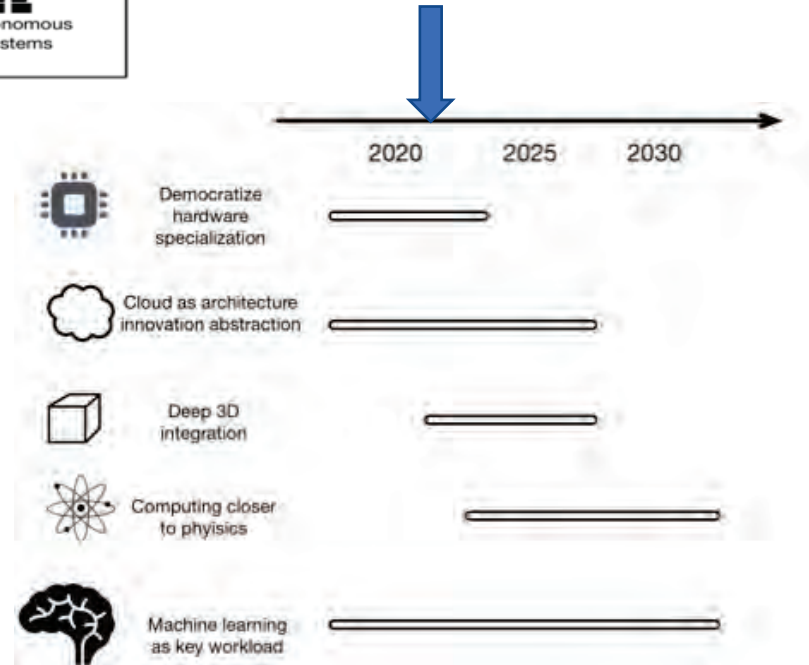
<https://www.karlrupp.net/2018/02/42-years-of-microprocessor-trend-data/>

I think most technologists will, at least privately, rationally consider the prospects for the end of Moore's Law. But they focus on the physics, which change substantially from one silicon process technology to the next. These technologists know how monumental the challenges are to even get to [7 nanometer] silicon technology, so the natural assumption is that eventually some problem with the next silicon process technology will turn out to be physically insurmountable, and that's what will end Moore's Law. They are right, there are very serious challenges looming, but then, the silicon industry has beaten back such challenges in the past. This gives a lot of people false confidence that we can do it again. My attitude is, maybe we can, maybe we can't, but physics isn't the only challenge. That was my point in focusing on economics, to remind the field that we have to succeed at the physics AND the economics or we will have failed, and Moore's Law will have ended.

Bob Caldwell/DARPA

In late 2016 the Computing Community Consortium released a workshop report considering future technological approaches to increasing computing performance

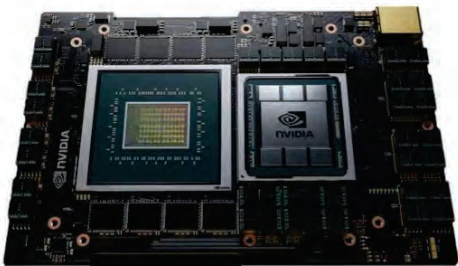
Arch2030: A Vision of Computer Architecture Research over the Next 15 Years



Hardware specialization and deep 3D integration yield breathtaking innovation

ANNOUNCING NVIDIA GRACE

Breakthrough CPU Designed for Giant-Scale AI and HPC Applications



FASTEST INTERCONNECTS
 >900 GB/s Cache Coherent NVLink CPU To GPU (14x)
 >600GB/s CPU To CPU (2x)

HIGHEST MEMORY BANDWIDTH
 >500GB/s LPDDR5x w/ ECC
 ~2x Higher B/W
 10x Higher Energy Efficiency

NEXT GENERATION ARM NEOVERSE CORES
 >300 SPECrate2017_int_base
 Availability 2023

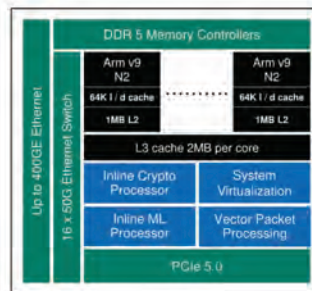


Intel
 Announces
 Sapphire
 Rapids
 with HBM,
 Reveals
 Ponte
 Vecchio
 Form
 Factors

Marvell Announces OCTEON 10 DPU Family: First to 5nm with N2 CPUs

by [Andrei Frumusanu](#) on June 28, 2021 6:30 AM EST

OCTEON 10 innovations



- 5nm TSMC process
 - Enables fanless designs
- First inline DPU ML Engine
- Hardware VPP acceleration
- Inline crypto processor
- Arm Neoverse N2 cores
 - Highest SPECint in industry
- PCIe 5.0, DDR5 support
- Integrated with 16x 50GE switch
- 56G SerDes

AMD-Xilinx Deal
 Gains UK, EU
 Approvals —
 China's Decision
 Still Pending
 By Todd R.
 Weiss/HPCWire
 July 1, 2021



Scientific community is deeply engaged in computing evolution and revolution

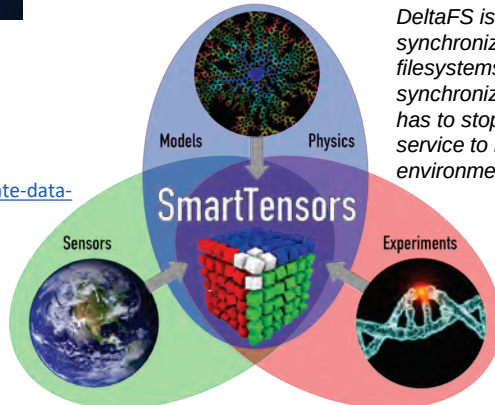


Credit: [Getty Images](#)

DNA: The Ultimate Data-Storage Solution

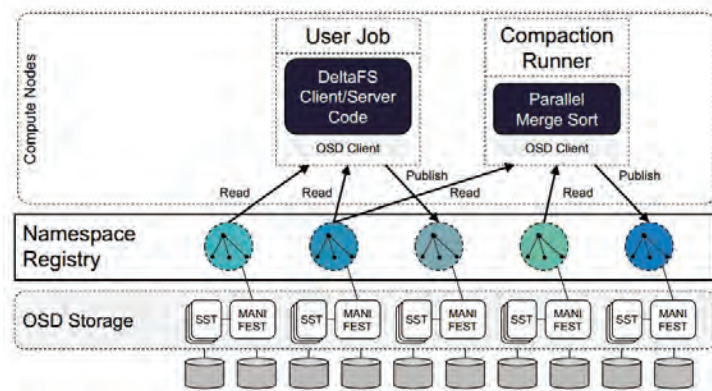
By [Latchesar Ionkov](#), [Bradley Settlemyer](#) on May 28, 2021

<https://www.scientificamerican.com/article/dna-the-ultimate-data-storage-solution/>



Unsupervised Physics-Informed Machine Learning of Complex Natural and Engineered Geoscience Processes

Los Alamos and Julia Computing will apply the Laboratory's novel, machine-learning software suite [SmartTensors](#) to identify patterns in massive geothermal and oil/gas datasets to discover hidden features by finding intrinsic similarities among the data elements. The team will develop a commercial framework for SmartTensors tailored toward natural and engineered geoscience applications that will facilitate extracting hidden signatures in geothermal and oil/gas datasets.



DeltaFS is based on the premise that at exascale and beyond, synchronization of anything global should be avoided. Conventional parallel filesystems, with fully synchronous and consistent namespaces, mandate synchronization with every file create and other metadata operations. This has to stop. Moreover, the idea of dedicating a single filesystem metadata service to meet the needs of all applications running on a single computing environment, is archaic and inflexible. This too must stop.

Advances in computing for national security have been built on decades of contributions from LANL in concert with industry



[Vector machine]



[SMP] [MPP/Data Parallel]



[Massively process parallel]



[commodity computing]



[Hybrid architecture]



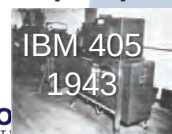
[Large core memory]



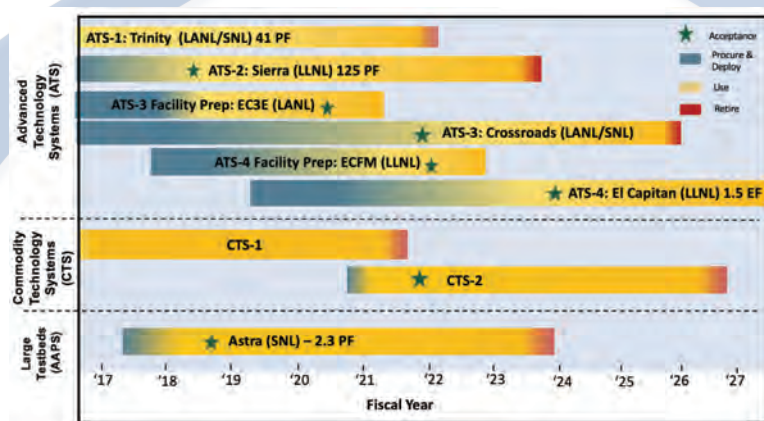
[Transistors]



[Tubes]



[Mechanical]



[Massive Memory / Burst Buffers]



[Quantum Annealing]



(App, Workflow, Code
Exploitation Efficiency)

HPC's role at the Lab has always been two-fold:

- Provide HPC to execute scientific mission
- Advance HPC to help execute future scientific mission

Thank you; upcoming speakers

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 - Leading development of LANL's AI vision, strategy and plan, IS&T Leadership Team