Sierra: The LLNL IBM CORAL System

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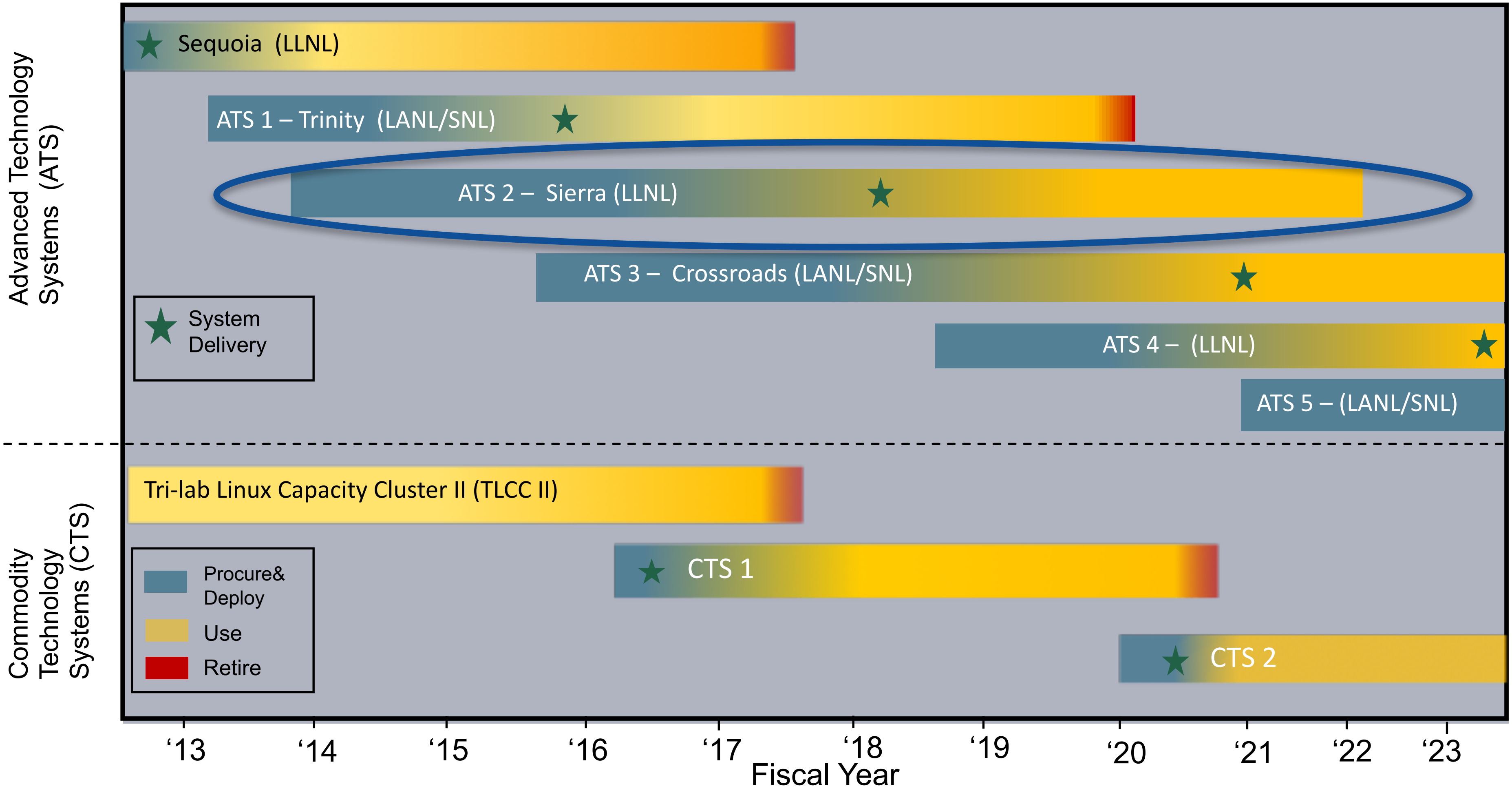
Sierra will be the next ASC ATS platform

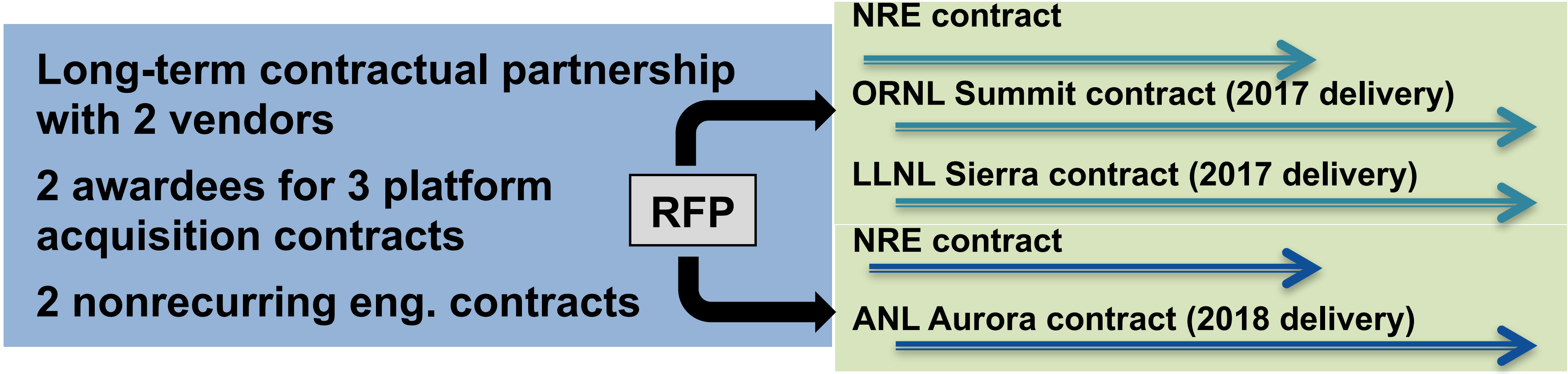


Sequoia and Sierra are the current and next-generation Advanced Technology Systems at LLNL

Sierra is part of CORAL, the Collaboration of Oak Ridge, Argonne and Livermore

Modeled on successful LLNL/ANL/IBM Blue Gene partnership (Sequoia/Mira)

LLNL's IBM Blue Gene Systems



Long-term contractual partnership with 2 vendors

2 awardees for 3 platform acquisition contracts

2 nonrecurring eng. contracts

RFP

NRE contract

ORNL Summit contract (2017 delivery)

LLNL Sierra contract (2017 delivery)

NRE contract

ANL Aurora contract (2018 delivery)

CORAL is the next major phase in the U.S. Department of Energy's scientific computing roadmap and path to exascale computing

The Sierra system that will replace Sequoia features a GPU-accelerated architecture

Compute Node

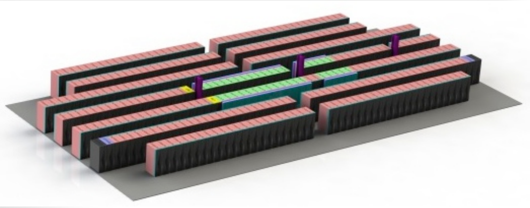
2 IBM POWER9 CPUs
4 NVIDIA Volta GPUs
NVMe-compatible PCIe 1.6 TB SSD
256 GiB DDR4
16 GiB Globally addressable HBM2 associated with each GPU
Coherent Shared Memory

Compute Rack

Standard 19”
Warm water cooling

Compute System

4320 nodes
1.29 PB Memory
240 Compute Racks
125 PFLOPS
~12 MW



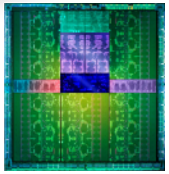
Components

IBM POWER9

- Gen2 NVLink

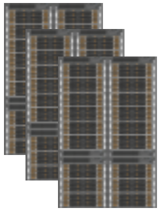
NVIDIA Volta

- 7 TFlop/s
- HBM2
- Gen2 NVLink



Mellanox Interconnect

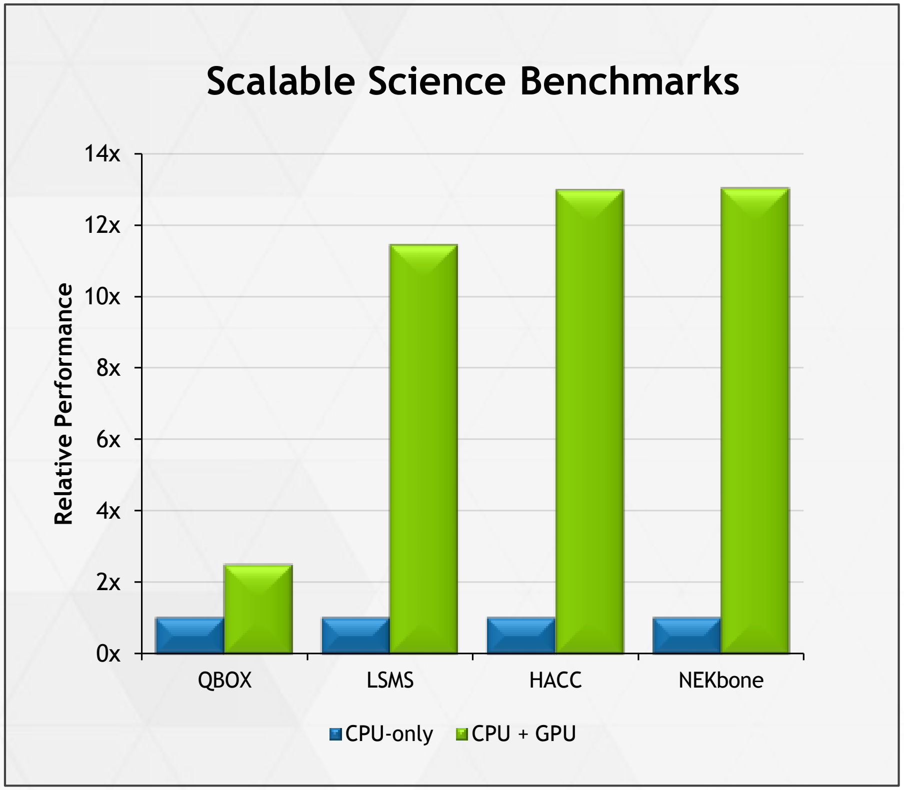
Single Plane EDR InfiniBand
2 to 1 Tapered Fat Tree

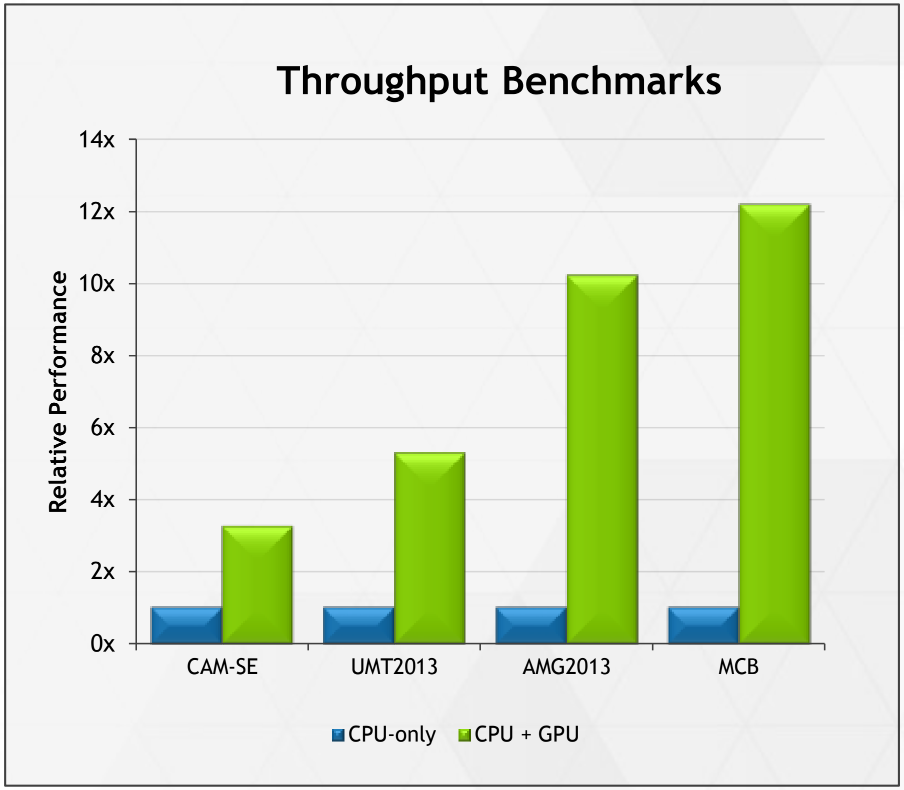


GPFS File System

154 PB usable storage
1.54 TB/s R/W bandwidth

Outstanding benchmark analysis by IBM and NVIDIA demonstrates the system's usability


Scalable Science Benchmarks


Throughput Benchmarks

Projections included code changes that showed tractable annotation-based approach (i.e., OpenMP) will be competitive

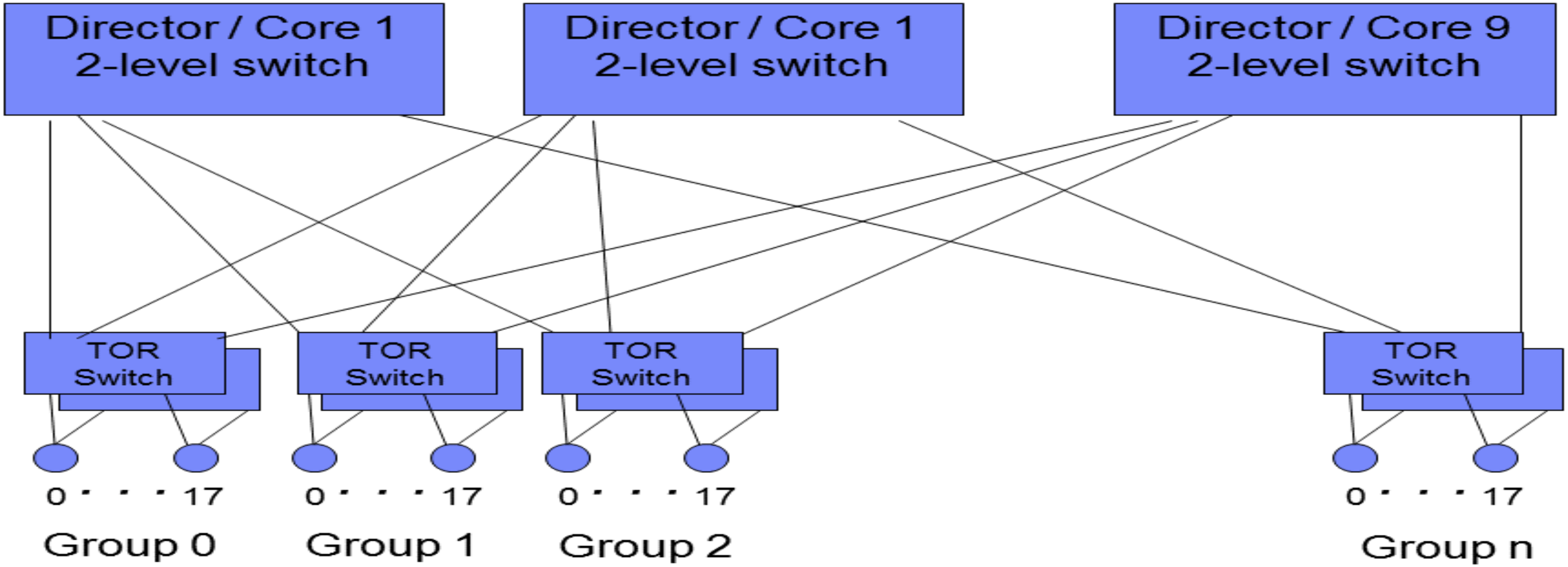
Sierra system architecture details have recently been finalized with Go decision

	Sierra	uSierra
Nodes	4,320	684
POWER9 processors per node	2	2
GV100 (Volta) GPUs per node	4	4
Node Peak (TFLOP/s)	29.1	29.1
System Peak (PFLOP/s)	125	19.9
Node Memory (GiB)	320	320
System Memory (PiB)	1.29	0.209
Interconnect	2x IB EDR	2x IB EDR
Off-Node Aggregate b/w (GB/s)	45.5	45.5
Compute racks	240	38
Network and Infrastructure racks	13	4
Storage Racks	24	4

These are working numbers; the final configuration will only be set once the system is fully installed

LLNL and ASC platform chose to use a tapered fat-tree for Sierra's network

- Full bandwidth from dual ported Mellanox EDR HCAs to TOR switches
- Half bandwidth from TOR switches to director switches
- An economic trade-off that provides approximately 5% more nodes


Director / Core 1
2-level switch

Director / Core 1
2-level switch

Director / Core 9
2-level switch

TOR Switch

TOR Switch

TOR Switch

TOR Switch

0 · · · 17

Group 0

0 · · · 17

Group 1

0 · · · 17

Group 2

0 · · · 17

Group n

This decision, counter to prevailing wisdom for system design, benefits Sierra's planned UQ workload: 5% more UQ simulations at performance loss of < 1%

Sierra architectural decisions reflect its planned UQ workload

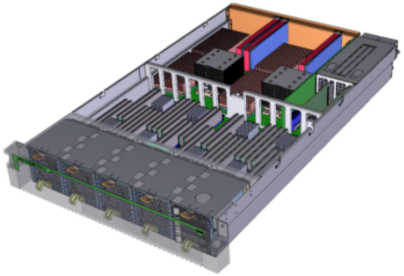
- Sierra is contrasted with ORNL's Summit system
  - Summit will feature 3 Voltas per Power9 (i.e., 6 GPUs per node)
  - Summit will provide a full bandwidth fat-tree
  - Summit will include 2X Sierra's main memory per node
- Sierra's workload will focus on uncertainty quantification
  - Multiphysics ensemble calculations that stress throughput
  - Will fit each physics package into 64 GiB memory (or less)
  - Aggregate memory footprint under reduced
  - Relatively low network demand, placed to minimize contention
- Sierra architectural decisions support this workload
  - Traded network and memory for compute nodes

These tradeoffs improve Sierra's effectiveness by about 5%

Early Access systems provide critical pre-Sierra generation resources

Early Access Compute Node

- “Minsky” HPC Server
- 2xPOWER8+ processors
- 4xNVIDIA GP100; NVLINK
- 256GB SMP (32x8GB DDR4)



Early Access Compute System

- 18 Compute Nodes
- EDR IB switch fabric
- Ethernet mgmt
- Air-cooled

Early Access to CORAL Software Technology

Based on IBM’s current technical programming offerings with enhancements for new function and scalability. Includes:

- Initial messaging stack implementation
- Initial Compute node kernel
- Compilers:
  - o Open Source LLVM
  - o PGI compiler
  - o XL compiler

Initial Early Access GPFS

- GPFS Management servers
- 2 POWER8 Storage controllers
- 1 GL-2; 2x58 6TB SAS drives or
- 1 GL-4; 4x58 6TB SAS drives
- EDR InfiniBand switch fabric

- Enhancement to GL-6, 6x58 6TB SAS drives in progress

Three LLNL Early Access systems support ASC and institutional preparations for Sierra

Compute | Compute | Infrastructure Storage

Shark
597.6TF

Manta
597.6 TF

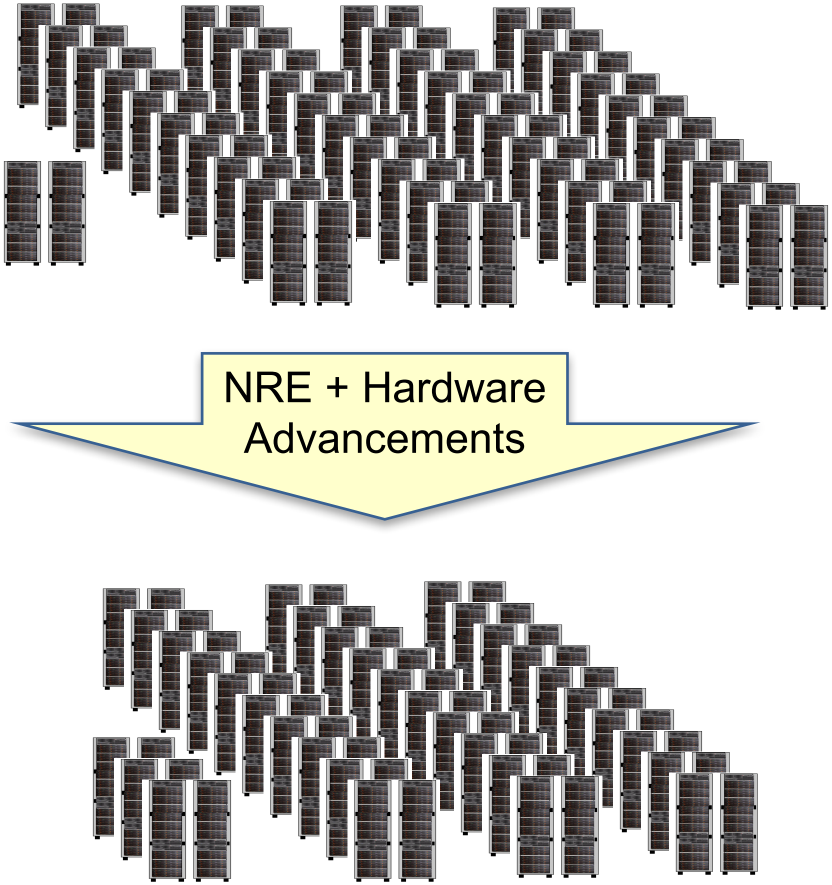
Compute | Compute | Infrastructure Storage

Compute nodes on Ray have 1.6TB NVMe drives →

Compute | Compute | Compute | Infrastructure | Storage

Ray:
896.4 TF

CORAL NRE drove Spectrum Scale advances that will vastly improve Sierra file system



Original Plan of Record

- 120PB delivered capacity
- Conservative drive capacity estimates
- 1TB/s write, 1.2TB/s read
- Concern about metadata targets

Modified (Cost Neutral)

- 154PB delivered capacity
- Substantially increased drive capacities
- 1.54 TB/s write/read
- Enhanced Spectrum Scale metadata perf. (many optimizations already released)

Close partnerships lead to ecosystem improvements

NVIDIA Volta GPUs (GV100) provide the bulk of Sierra's compute capability

SMs	80
FP64 Units (per SM)	32
FP32 Units (per SM)	64
Tensor Cores (per SM)	8
Register File (per SM)	256KiB
L1/Shared Memory (per SM)	128KiB
Double Precision Peak (TFlop/s)	7 (7.5)
Single Precision Peak (TFlop/s)	14 (15)
Tensor Op Peak (TOp/s)	120
HBM2 Bandwidth (GB/s)	898
NVLINK BW to CPU/Other GPU	75 (60)

To realize Sierra's full potential, we must exploit the tensor operations. The commoditization of machine learning will make this an enduring challenge.

Jeff Hittinger’s LDRD team is exploring techniques to exploit capabilities in traditional simulations

Task-based mixed precision

Multilevel representation

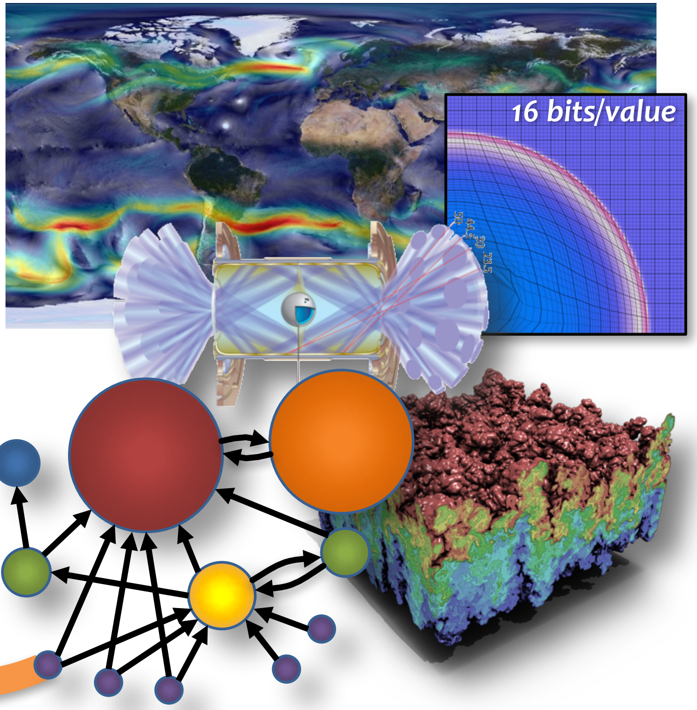
Libraries and Tools

Adaptive-rate compression

New number representations

ARM / Commodity GPU cluster

Applications

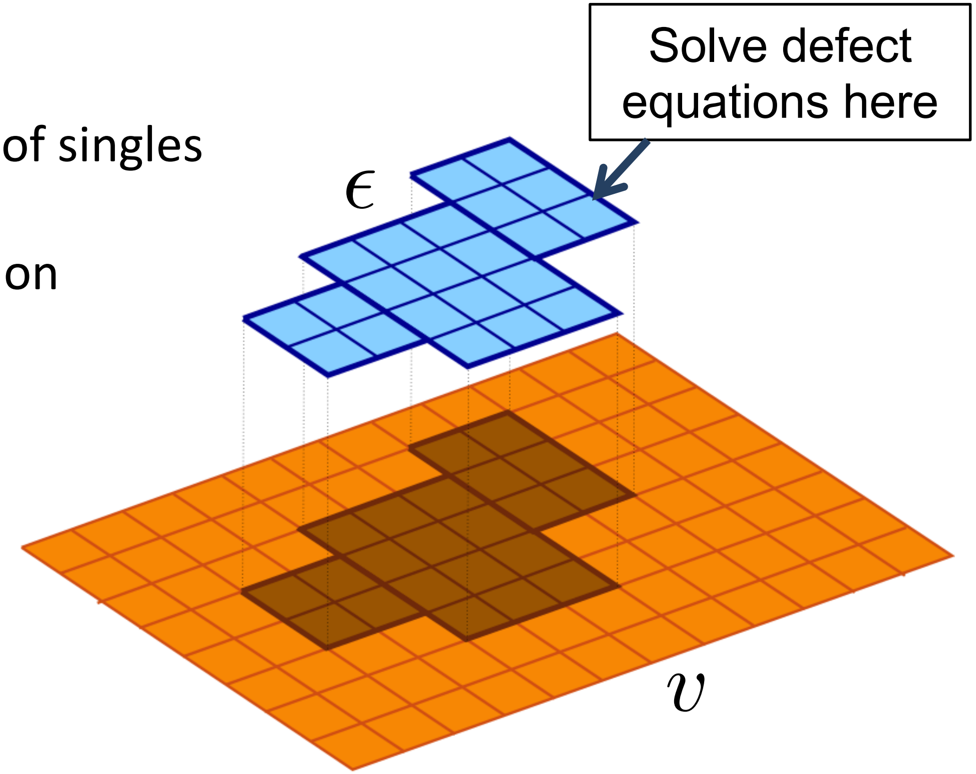


Success requires close collaboration with applications

A promising direction is the potential for an AMR-like dynamic, local mixed precision

- **Dynamic Mixed Precision**
  - Hierarchical representation: sum of singles
  - Block-based refinement
  - Most calculations in single precision
  - Key issues
    - Refinement criteria
    - Propagation of round-off error
    - Cost/benefit

- **Error transport techniques to understand error evolution:**

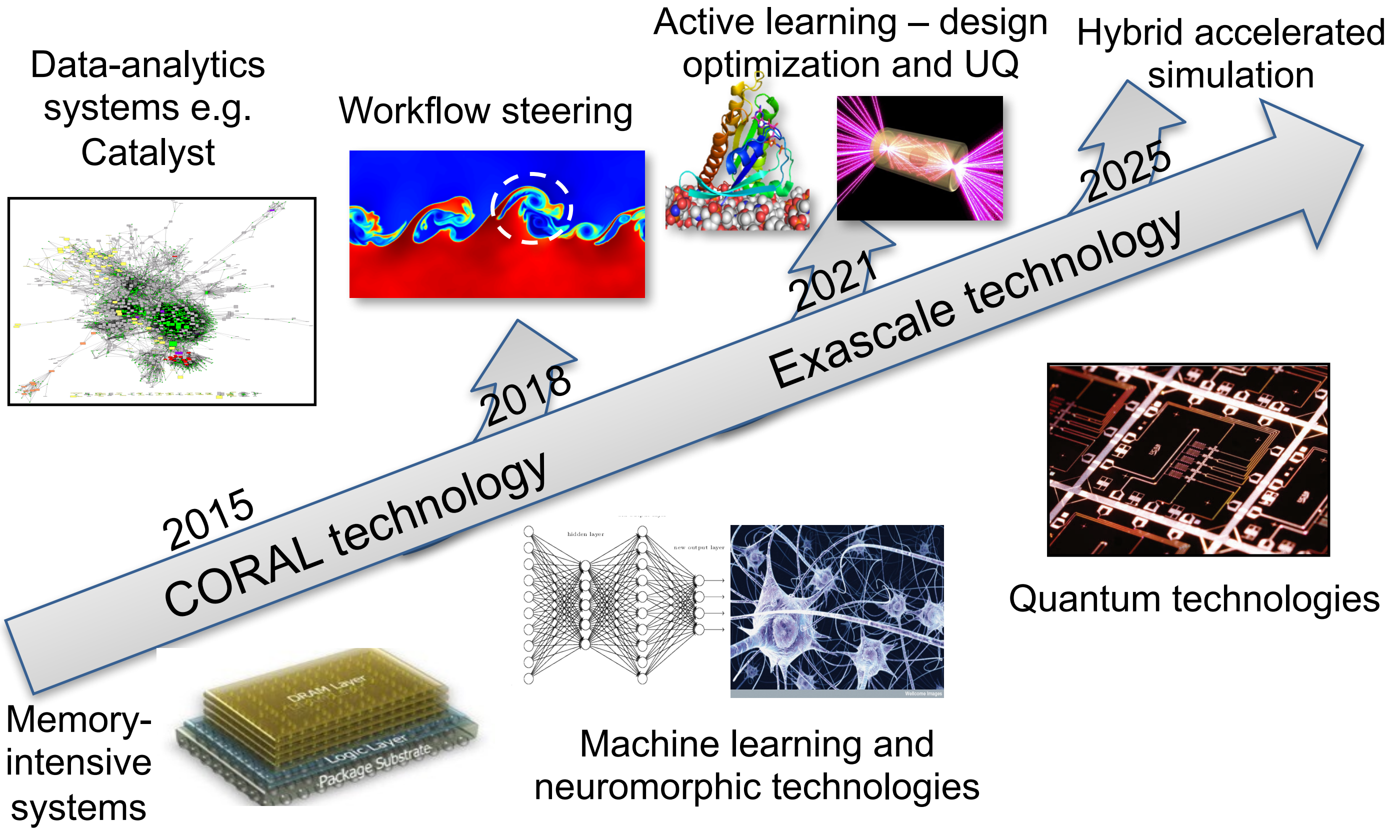


Solve defect equations here

$$\underbrace{u}_{\texttt{double}} = \underbrace{v}_{\texttt{single}} + \underbrace{\epsilon^{(0)}}_{\texttt{single}} + \underbrace{\epsilon^{(1)}}_{\texttt{single}} + \cdots$$

Advanced technology insertion will establish new directions for high-performance computing

Analytics and simulation convergence ⇨ **Cognitive simulation systems**



Data-analytics systems e.g. Catalyst

Workflow steering

Active learning – design optimization and UQ

Hybrid accelerated simulation

2015

2018

2021

2025

CORAL technology

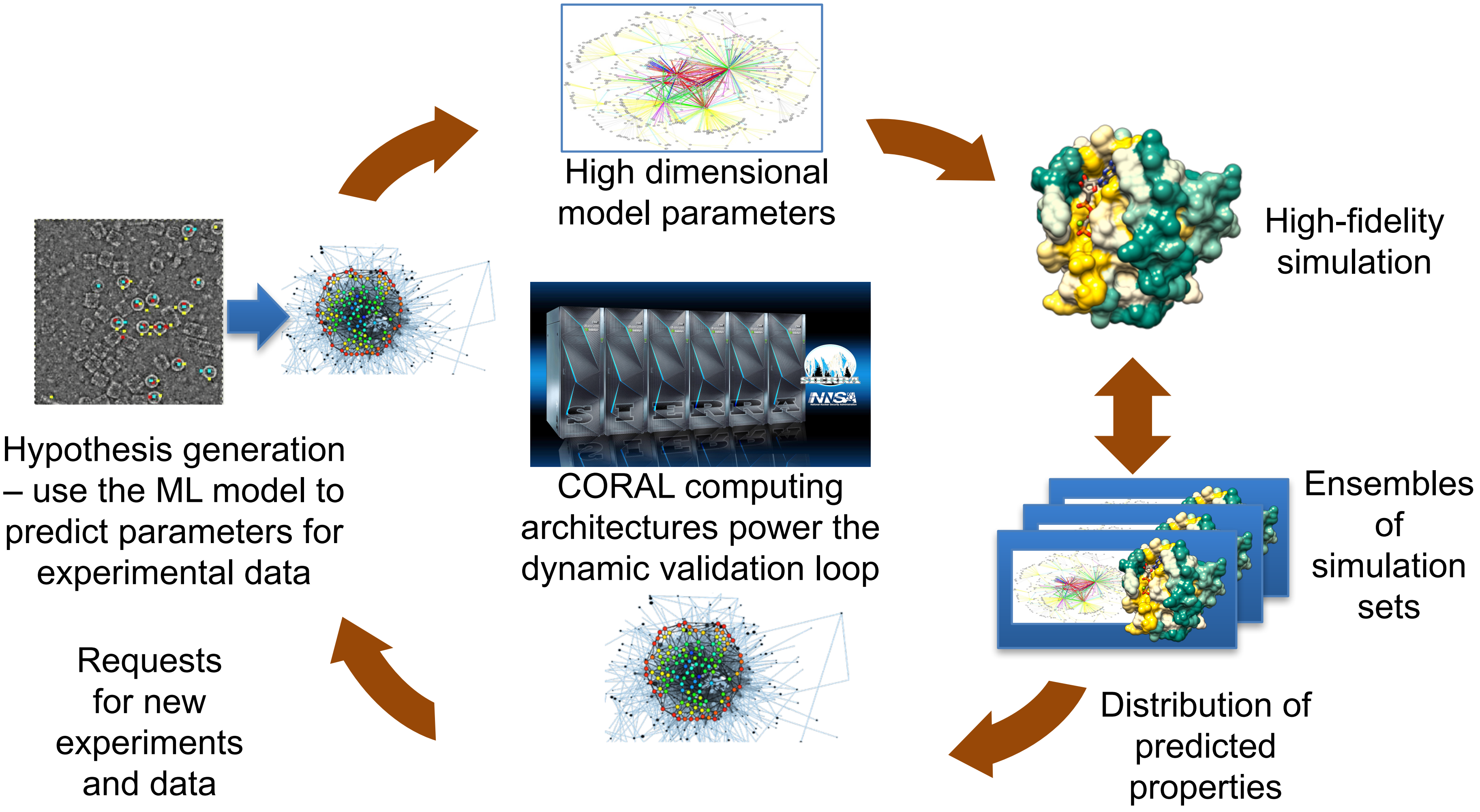
Exascale technology

Memory-intensive systems

Machine learning and neuromorphic technologies

Quantum technologies

Integrated machine learning and simulation could enable dynamic validation of complex models



High dimensional
model parameters

High-fidelity
simulation

Ensembles
of
simulation
sets

Distribution of
predicted
properties

Requests
for new
experiments
and data

Hypothesis generation
– use the ML model to
predict parameters for
experimental data

CORAL computing
architectures power the
dynamic validation loop

Sierra and its EA systems are beginning an accelerator-based computing era at LLNL

- The advantages that led us to select Sierra generalize
  - Power efficiency
  - Network advantages of "fat nodes"
  - Balancing capabilities/costs implies complex memory hierarchies
- Planning a similar, unclassified, M&IC resource
  - Same architecture as Sierra
  - Up to 25% of Sierra's capability
- Exploring possibilities for other GPU-based resources
  - Not necessarily NVIDIA-based
  - May support higher single precision performance

We have multiple projects planned to foster a healthy ecosystem

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