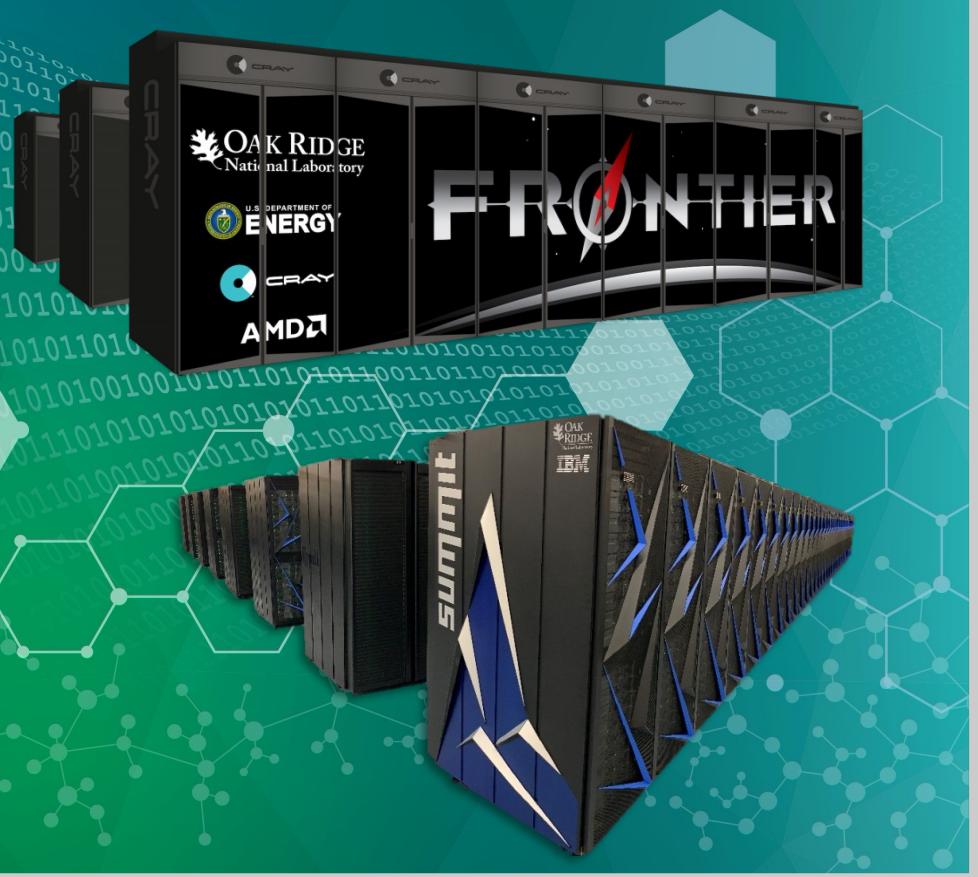
OAK RIDGE National Laboratory

OLCF: From Summit to Frontier

ATPESC – August 1, 2022



Tom Papatheodore

HPC Engineer

System Acceptance & User Environment

Oak Ridge Leadership Computing Facility (OLCF)

ORNL is managed by UT-Battelle LLC for the US Department of Energy

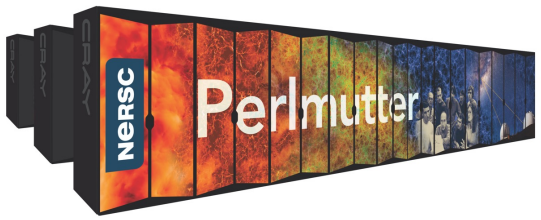
U.S. DEPARTMENT OF ENERGY

DOE's Office of Science Computation User Facilities

NERSC

Argonne NATIONAL LABORATORY Leadership Computing Facility

OAK RIDGE National Laboratory LEADERSHIP COMPUTING FACILITY



Perlmutter: ~100 PF

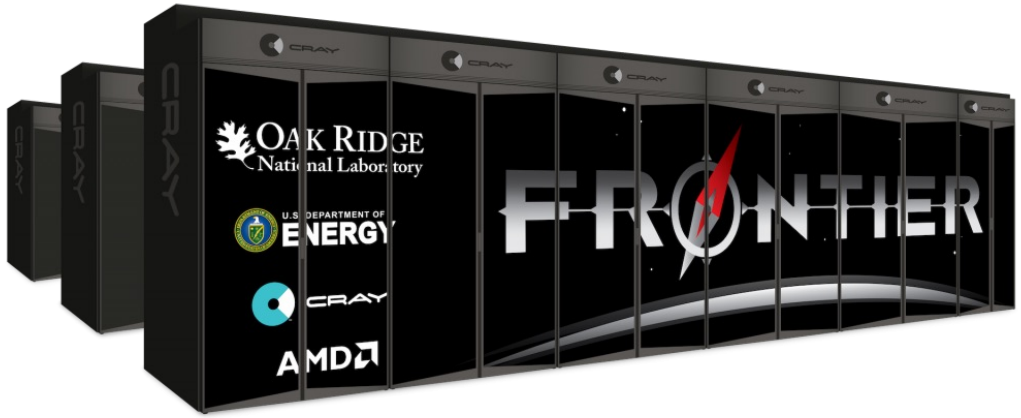
Aurora: >2 EF

Frontier: ~2 EF

- DOE is leader in open High-Performance Computing
- Provide the world's most powerful computational tools for open science
- Access is free to researchers who publish
- Boost US competitiveness
- Attract the best and brightest researchers

What is a Leadership Computing Facility (LCF)?

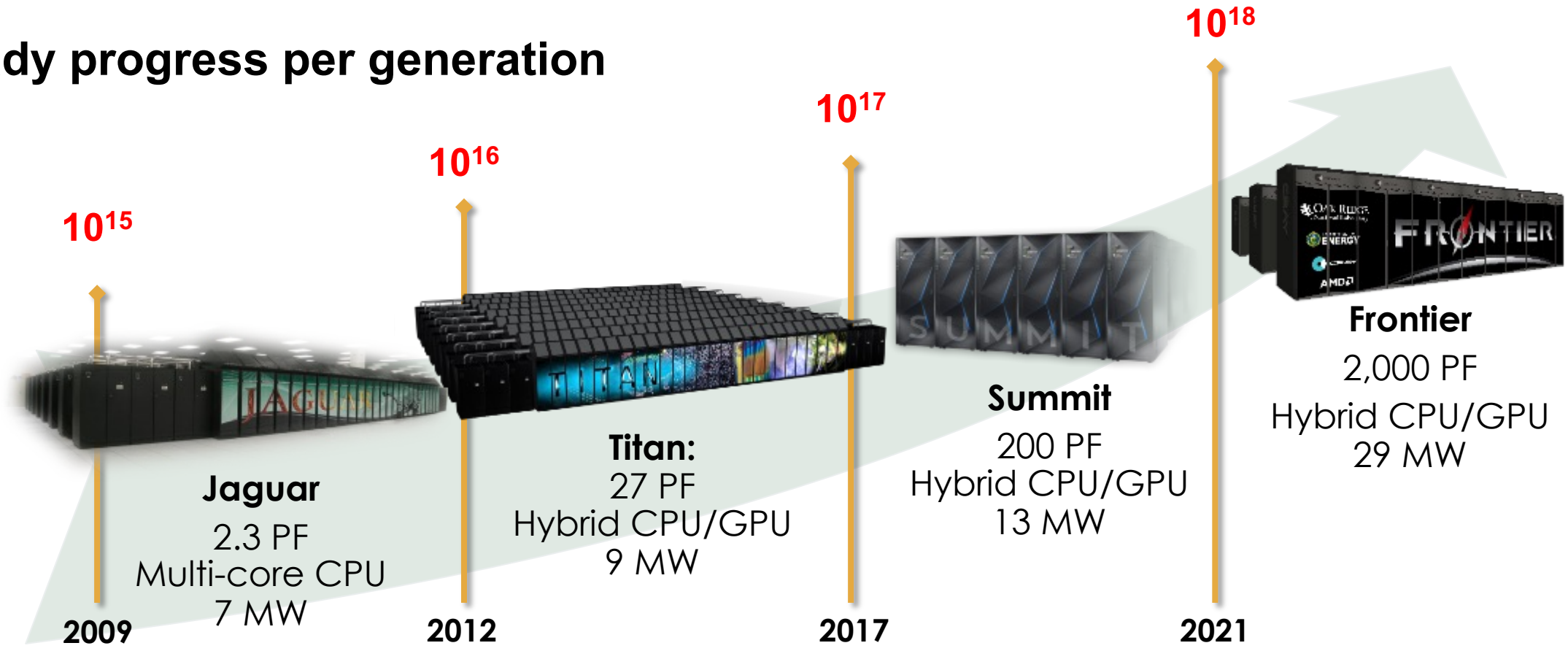
- Collaborative DOE Office of Science user-facility program at ORNL and ANL
- Mission: Provide the computational and data resources required to solve the most challenging problems.
- 2-centers/2-architectures to address diverse and growing computational needs of the scientific community
- Highly competitive user allocation programs (INCITE, ALCC).
- Projects receive 10x to 100x more resource than at other generally available centers.
- LCF centers partner with users to enable science & engineering breakthroughs (Liaisons, Catalysts).



From Petascale to Exascale

Mission: Providing world-class computational resources and specialized services for the most computationally intensive global challenges	Vision: Deliver transforming discoveries in energy technologies, materials, biology, environment, health, etc.

Steady progress per generation



OLCF's Summit Supercomputer (#4 June22 Top500 List)

OLCF Summit Overview

The system includes

- 4,680 nodes
- Dual-port Mellanox EDR InfiniBand network
- 250 PB IBM file system transferring data at 2.5 TB/s

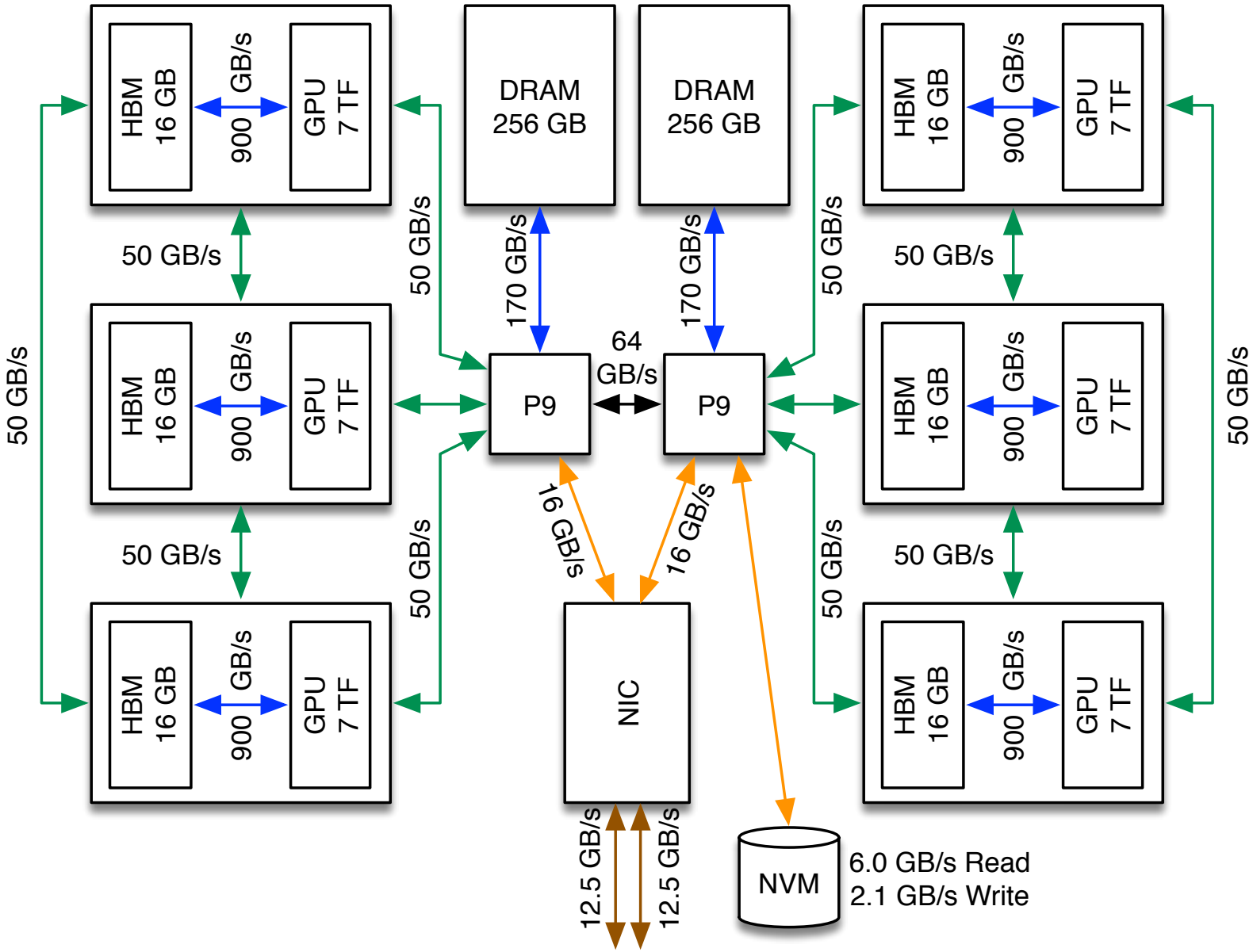
System Performance

- Peak of 200 Petaflops (FP_{64}) for modeling & simulation
- Peak of 3.3 ExaOps (FP_{16}) for data analytics and artificial intelligence

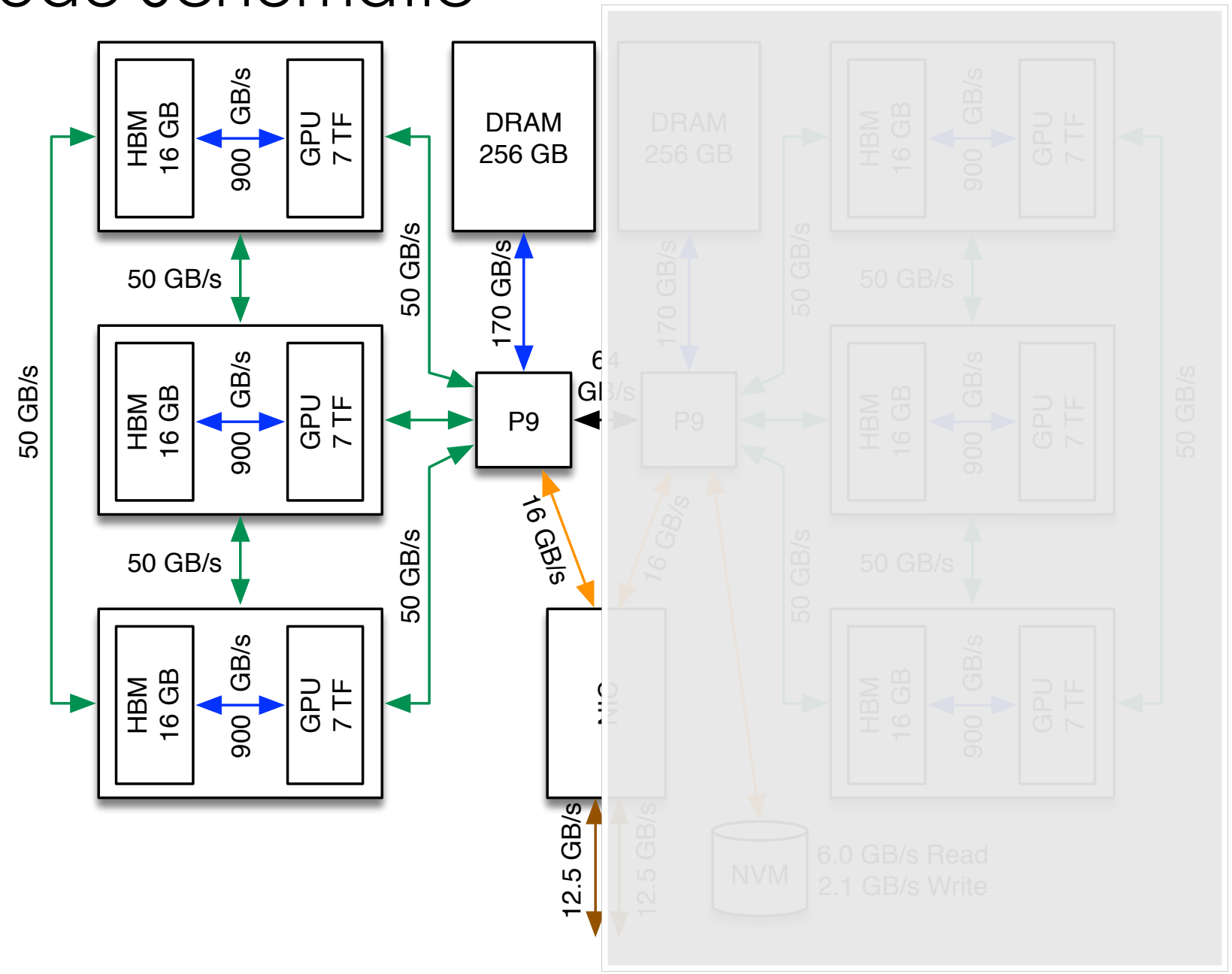
Each node has

- 2 IBM POWER9 processors
- 6 NVIDIA Tesla V100 GPUs
- 608 GB of fast memory (96 GB HBM2 + 512 GB DDR4)
- 1.6 TB of NV memory

Summit Node Schematic

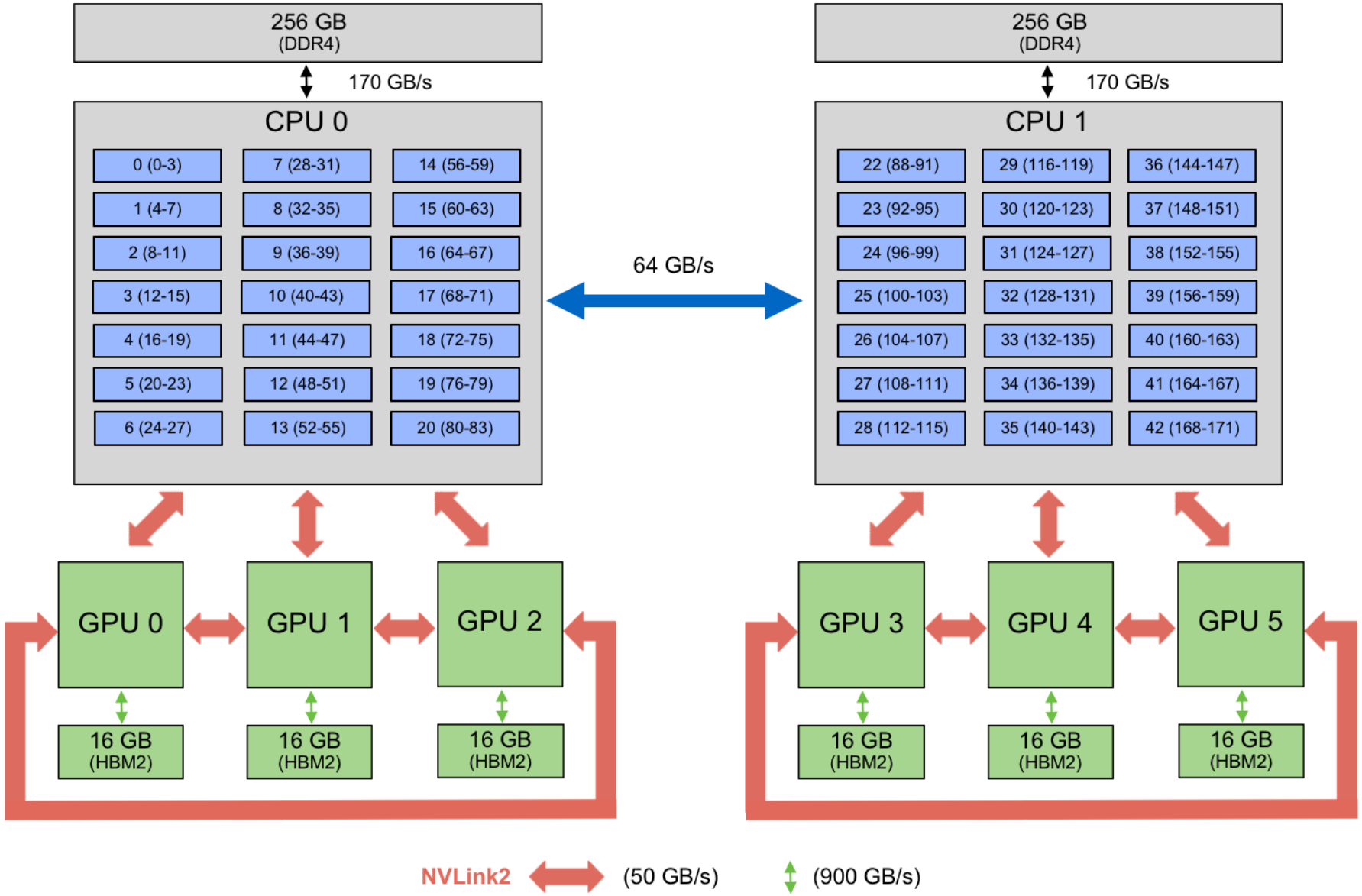


Summit Node Schematic

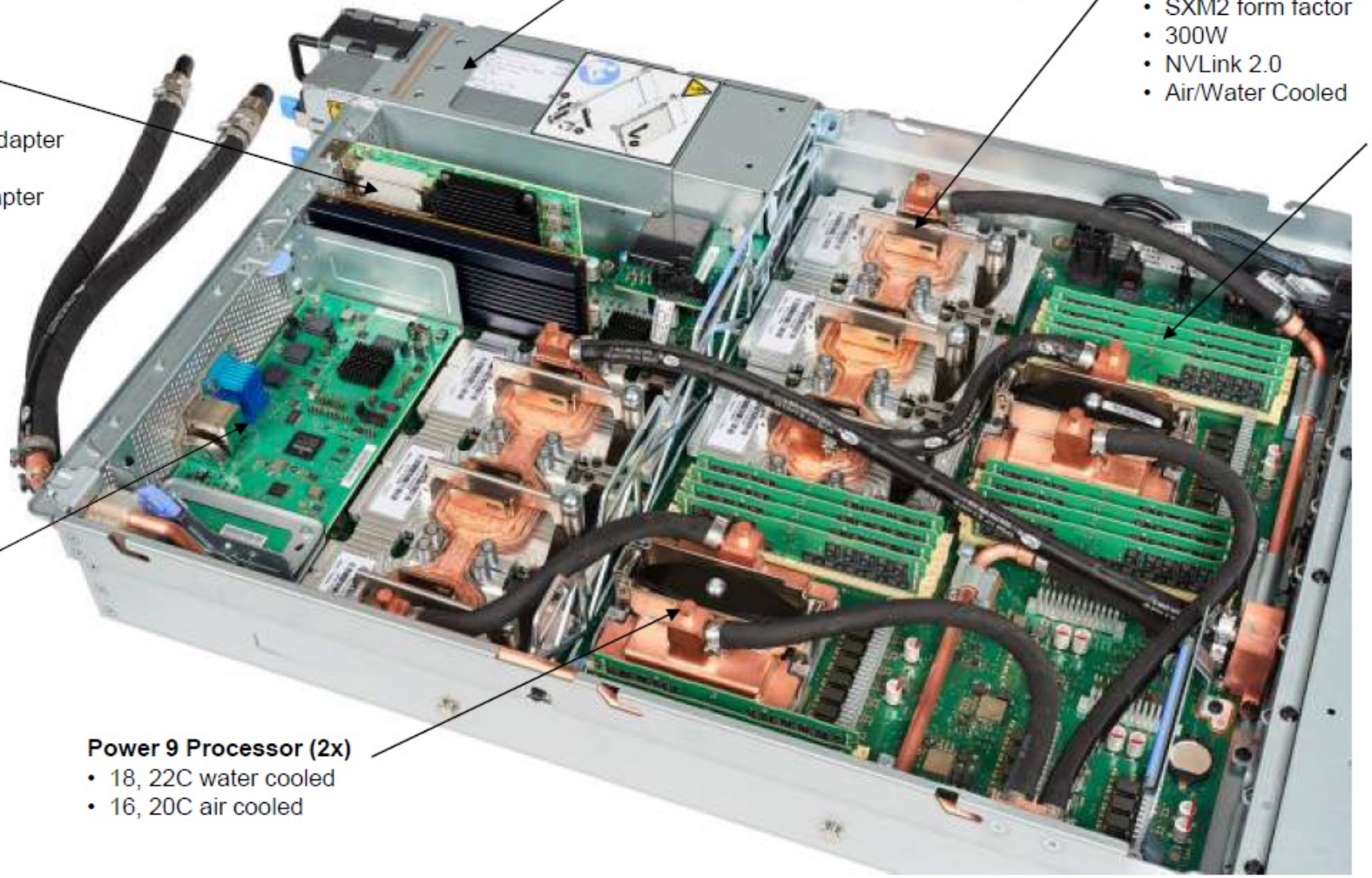


Summit Node

(2) IBM Power9 + (6) NVIDIA Volta V100



Summit Board (1 node) showing the Water Cooling



Power Supplies (2x)
- 2200W
- 200VAC, 277VAC, 400VDC input

NVidia Volta GPU
- 3 per socket
- SXM2 form factor
- 300W
- NVLink 2.0
- Air/Water Cooled

PCIe slot (4x)
- Gen4 PCIe
- 2, x16 HHHL Adapter
- 1, Shared slot
- 1 x8 HHHL Adapter

Memory DIMM's (16x)
- 8 DDR4 IS DIMMs per socket
- 8, 16, 32,64, 128GB DIMMs

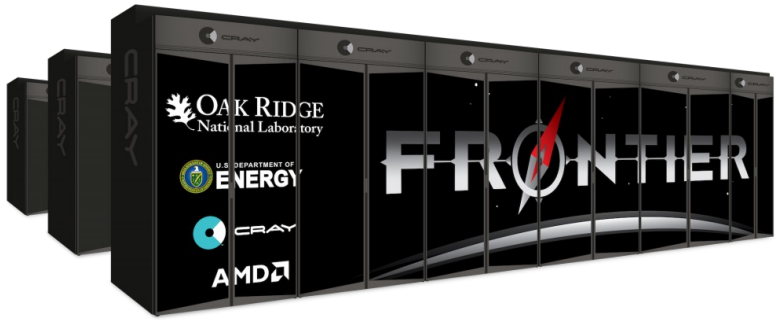
BMC Card
- IPMI
- 1 Gb Ethernet
- VGA
- 1 USB 3.0

Power 9 Processor (2x)
- 18, 22C water cooled
- 16, 20C air cooled

OLCF's Frontier Supercomputer (#1 June22 Top500 List)

Frontier Overview

Extraordinary Engineering



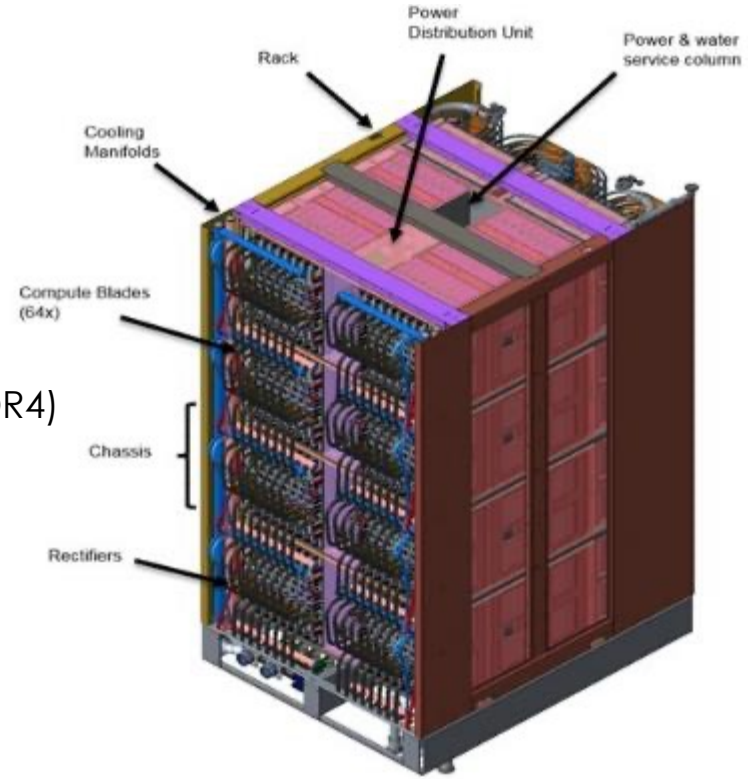
System

- 2.0 EF Peak DP FLOPS
- 74 compute racks
- 29 MW Power Consumption
- 9,408 nodes
- 9.2 PiB memory (4.6 PiB HBM, 4.6 PiB DDR4)
- Cray Slingshot network with dragonfly topology
- 37 PB Node Local Storage
- 716 PB Center-wide storage
- 4,000 ft^2 footprint

Built by HPE

Olympus rack

- 128 AMD nodes
- 8,000 lbs
- Supports 400 KW



Powered by AMD

AMD node

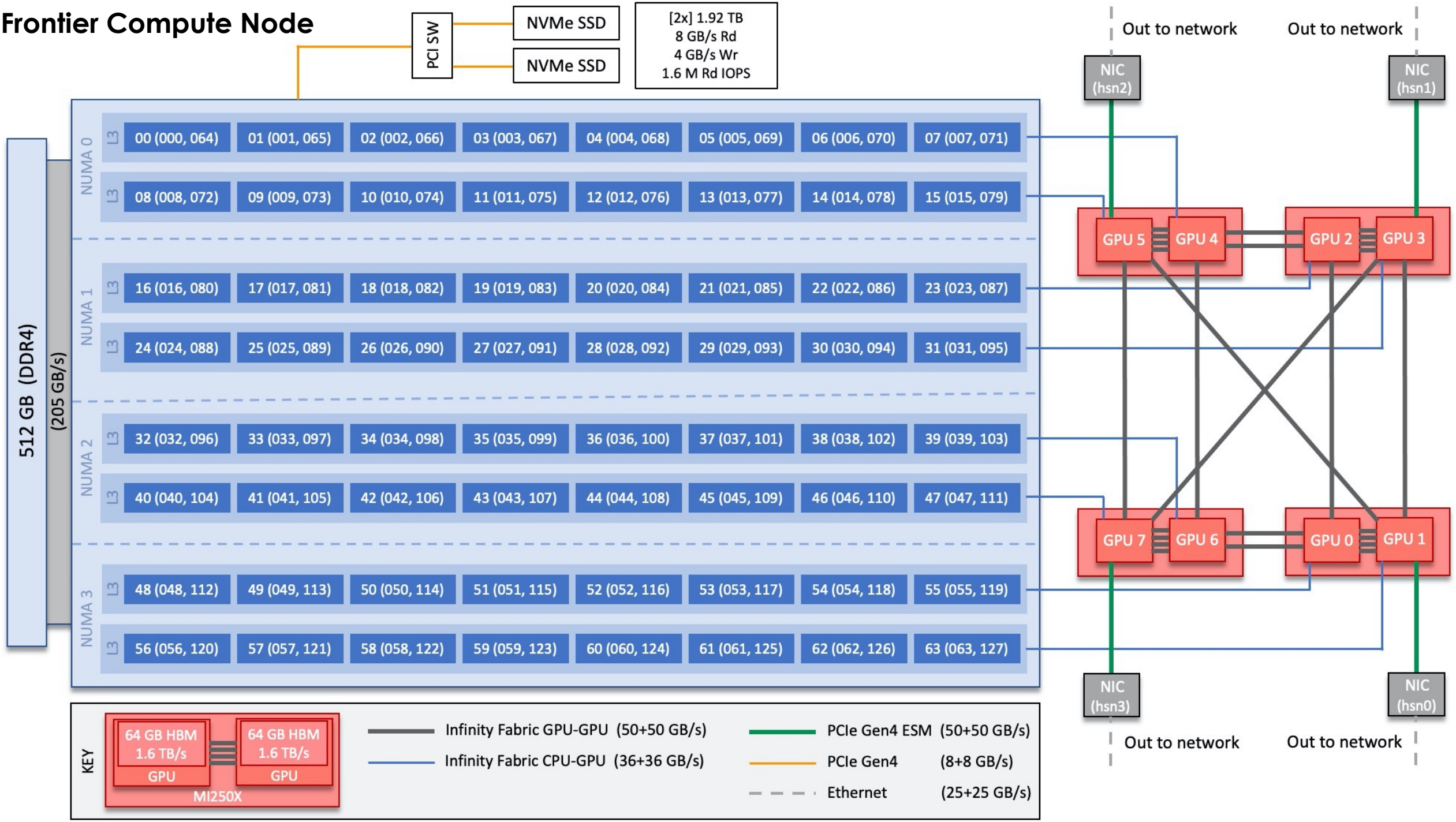
- 1 AMD "Optimized 3rd Gen EPYC" CPU
- 4 AMD MI250X GPUs
- 512 GiB DDR4 memory on CPU
- 512 GiB HBM2e total per node
  (128 GiB HBM per GPU)
- Coherent memory across the node
- 4 TB NVM
- GPUs & CPU fully connected with AMD Infinity Fabric
- 4 Cassini NICs, 100 GB/s network BW

Compute blade

- 2 AMD nodes

All water cooled, even DIMMS and NICs

Frontier Compute Node



OLCF Supercomputers: 2 Generations Later

- One cabinet of Frontier has a 10% higher HPL than all of Titan
  - While only using 309 kW compared to the Titan's 7 MW

One Cabinet
24 ft^2

>

200 Cabinets
~4,500 ft^2

OLCF Systems by the numbers

System	Titan (2012)	Summit (2017)	Frontier (2021)
Peak	27 PF	200 PF	2.0 EF
# nodes	18,688	4,608	9,408
Node	1 AMD Opteron CPU 1 NVIDIA Kepler GPU	2 IBM POWER9™ CPUs 6 NVIDIA Volta GPUs	1 AMD EPYC "Trento" CPU 4 AMD Instinct MI250X GPUs
Memory	0.6 PB DDR3 + 0.1 PB GDDR	2.4 PB DDR4 + 0.4 HBM + 7.4 PB NVM	4.6 PB DDR4 + 4.6 PB HBM2e + 36 PB NVM
On-node interconnect	PCI Gen2 – no coherence across the node	NVIDIA NVLINK - coherent memory across the node	AMD Infinity Fabric - coherent memory across the node
System Interconnect	Cray Gemini network 6.4 GB/s	Mellanox Dual-port EDR IB 25 GB/s	Four-port Slingshot network 100 GB/s
Topology	3D Torus	Non-blocking Fat Tree	Dragonfly
Storage	32 PB, 1 TB/s, Lustre Filesystem	250 PB, 2.5 TB/s, IBM Spectrum Scale™ with GPFS™	695 PB HDD+11 PB Flash Performance Tier, 9.4 TB/s and 10 PB Metadata Flash, Lustre
Power	9 MW	13 MW	29 MW
CPU:GPU	1:1	1:3	1:8
CPU Mem BW	50 GB/s	170 GB/s per CPU	205 GB/s
GPU Mem BW	1x 250 GB/s 250 GB/s Total	3x 900 GB/s 2,700 GB/s Total	8x 1,635 GB/s 13,080 GB/s Total
Interconnect BW	1x 8 GB/s 8 GB/s Total	3x 50 GB/s 150 GB/s Total	8x 36 GB/s 288 GB/s Total
Fast-to-Slow Memory Ratio	~~5:1 GPU:CPU~~ 32:1 GPU:CPU limited by PCIe	16:1 not limited by NVLink	64:1 not limited by xGMI-2

Frontier Programming Environment

Vendor-Provided

- Cray Programming Environment (CPE)
  - Cray, AMD, GCC compilers
  - Cray profiling, tuning, debugging tools
  - CrayMPI optimized for AMD GPU direct
- AMD ROCm programming environment
  - Support for HIP and GPU offload

Other Sources

- ECP
  - LLVM enhancements: Flang (front-end), OpenMP/ACC
  - Kokkos, RAJA, HIP LZ (HIP support for Aurora)
  - MPI, HPCToolkit, PAPI enhancements, …
- OLCF
  - Pilot implementation: DPC++/SYCL for Frontier (+ALCF)
  - GCC enhancements: OpenACC, OpenMP, Fortran

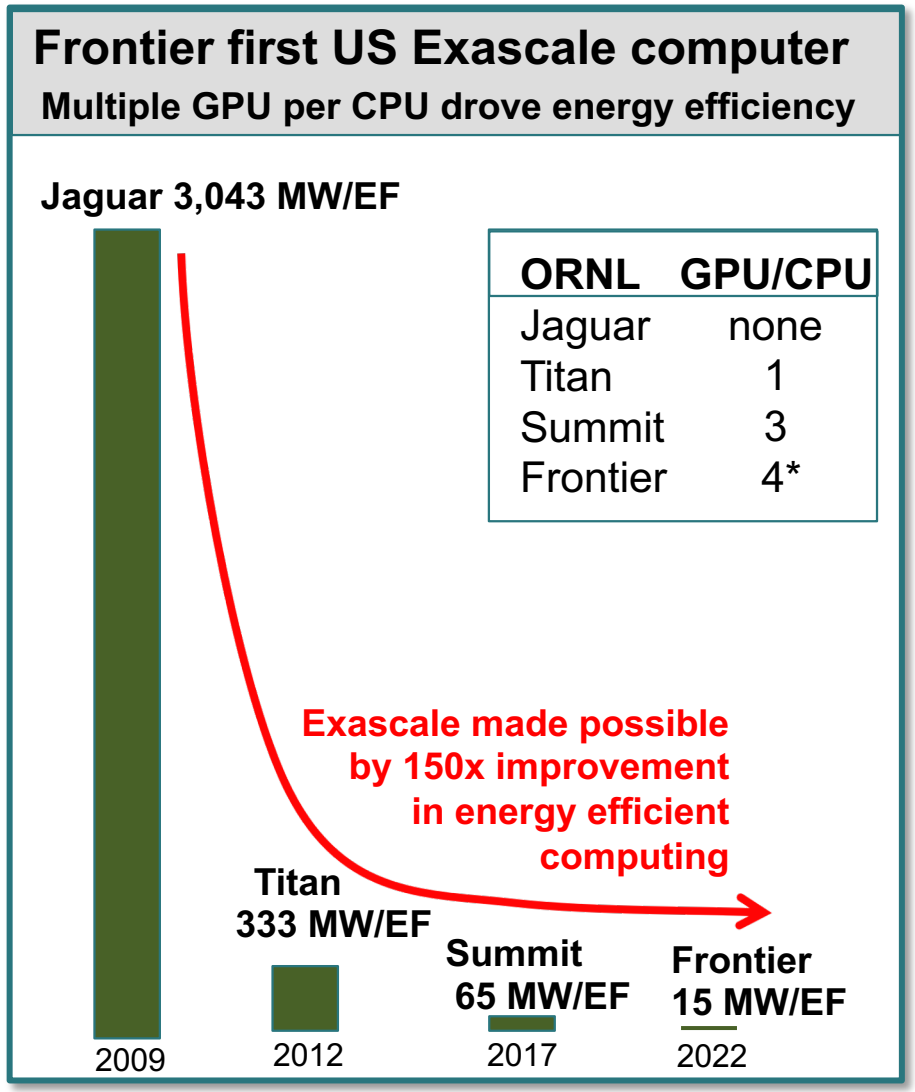
- Compilers Offered: Cray PE (C/C++ LLVM-based; Cray Fortran), AMD ROCm (LLVM-based), GCC
- Programming Languages/Models Supported (in which compilers)
  - C, C++, Fortran (all)
  - OpenACC (GCC; 2.6 substantially complete, 2.7 planned)
  - OpenMP (all; 5.0-5.2 in progress – most priority features complete, details vary)
  - HIP (Cray, AMD; semi-automatic translation from CUDA to HIP via hipify tools)
    (CUDA Fortran: HIP kernels called from Fortran)
  - Kokkos/RAJA (all)
  - UPC (Cray, GCC)

Items in green are also available on Summit

Energy Efficiency - One of the key Exascale challenges

Since 2008, one of the biggest concerns with reaching Exascale has been energy consumption

- **ORNL pioneered GPU use in supercomputing** beginning in 2012 with Titan thru today with Frontier. Significant part of energy efficiency improvements.
- **DOE *Forward vendor investments** in energy efficiency (2012-2020) further reduced the power consumption of computing chips (CPUs and GPUs).
- **150x reduction in energy per FLOPS** from Jaguar to Frontier at ORNL
- ORNL achieves additional energy savings from using warm water cooling in Frontier (32 C).
  ORNL Data Center PUE= 1.03



Questions?

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