OAK RIDGE National Laboratory

Frontier

2025-07-28 - Argonne Training Program on Extreme-Scale Computing (ATPESC)

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HPC Engineer, System Acceptance & User Environment

Oak Ridge Leadership Computing Facility

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

U.S. DEPARTMENT OF ENERGY

What is a Leadership Computing Facility (LCF)?

- Partner with users to enable science and engineering breakthroughs
- Mission: Provide capability computing resources for the most difficult problems
- Resources are unique scientific instruments
  - Closer in use, intent, purpose, and scale to Large Hadron Collider and James Webb telescope than your laptop
- Allow users to investigate otherwise inaccessible systems across scales
  - Galaxy Formation to Nanomaterials

https://www.flickr.com/photos/olcf/52117623798

https://www.chicagomag.com/wp-content/uploads/2023/01/C202302-Aurora-Supercomputer-nodes.jpg

Who Uses Leadership Computing Facilities?

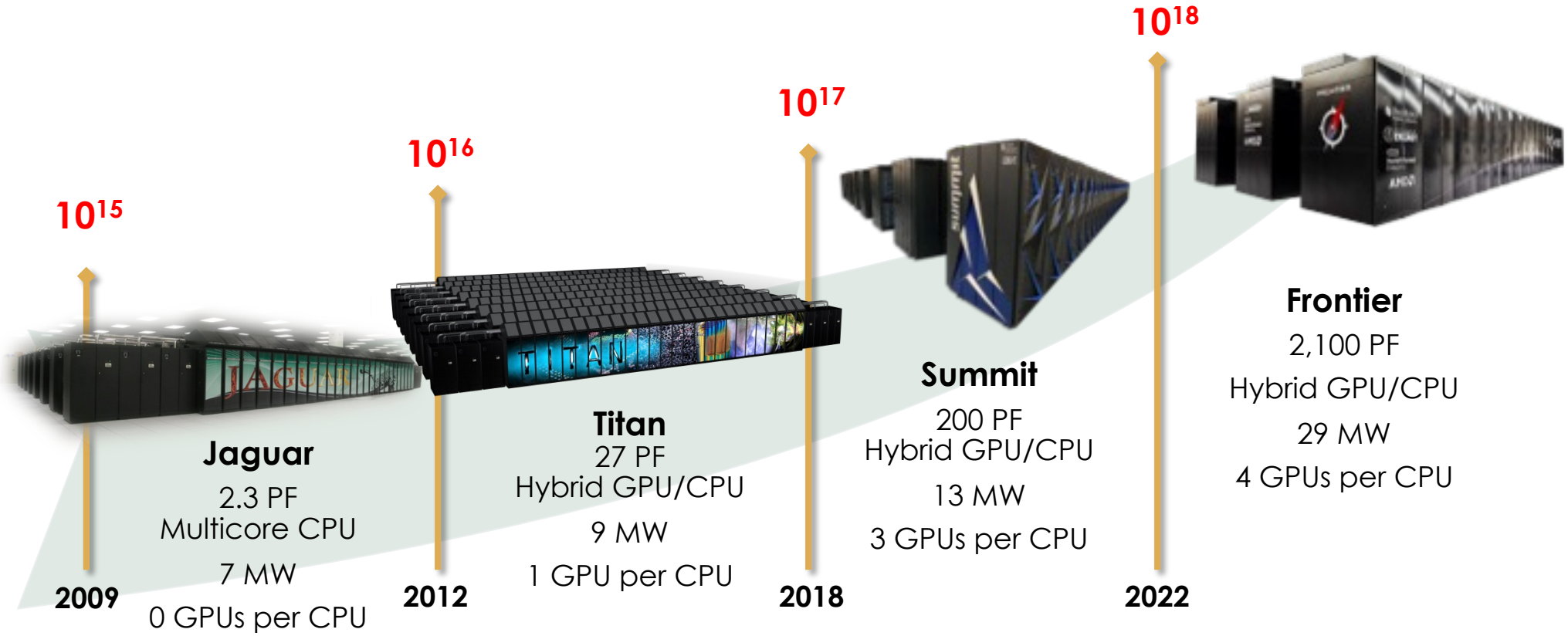
- Users from across the world
  - Academia, industry, national laboratories
- Time awarded through allocation programs
  - INCITE (Large)
    - Innovative and Novel Computational Impact on Theory and Experiment Program
  - ALCC (Small-Medium)
    - ASCR Leadership Computing Challenge
  - DD (Small)
    - Director's Discretionary
  - OLCF Pathways to Supercomputing Initiative (Startup)
    - Time and staff support to prepare for larger allocations

Oak Ridge Leadership Computing Facility (OLCF)

- One of two Department of Energy LCFs
- Based in Oak Ridge, TN at the Oak Ridge National Laboratory (ORNL)
- Department of Energy-funded research
  - Neutron Science, High-Performance Computing, Advanced Materials, Biology and Environmental Science, Nuclear Science and Engineering, Isotopes, and National Security
- Largest, most modern center for unclassified computing in the US

https://www.ornl.gov/sites/default/files/styles/basic_page_hero/public/2008-P01679.jpg

From Petascale to Exascale



A Note on Energy Efficiency

- 145x reduction in energy per FLOPS from Jaguar to Frontier
  - 3,043 MW/EF in 2009 -> 21 MW/EF in 2022
- 1 Frontier cabinet has 10% more performance than all of Titan
  - Using 309 kW compared to Titan's 9 MW

1 Frontier Cabinet (2022)

200 Titan Cabinets (2012)

Frontier System Overview

- HPE Cray EX Supercomputer architecture
  - 9,856 compute nodes across 77 cabinets
  - 2.1 EF peak double-precision performance
    - 1.102 EF HPL performance (June 2022 debut)
    - 1.353 EF HPL performance(June 2025)
  - AMD 64-core Optimized 3rd Gen EPYC CPUs
  - AMD Instinct MI250X GPUs
  - HPE Slingshot interconnect
  - Cray and AMD ROCm prog. environments
  - 679 PB Lustre filesystem, "Orion"
  - NFS storage (/ccs/home, etc.)

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HPE Cray EX4000 Cabinet

- 8x compute chassis per cabinet
  - Up to 64x compute blades
  - Up to 64x HPE Slingshot switch blades
- Direct liquid cooling using a shared Coolant Distribution Unit (CDU)
- 4x power shelves with a max of 8x rectifiers each
- Supports 400 kW

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HPE Cray EX4000 Cabinet

- 8x compute chassis per cabinet
  - 8x compute blades per chassis
  - 4x switch blades per chassis
- Frontier cabinets consist of:
  - 64x compute blades
  - 128x compute nodes
  - 512x network interface cards (NIC)
  - 32x HPE slingshot switches
  - 1x Dragonfly group
- 8,000 pounds per cabinet

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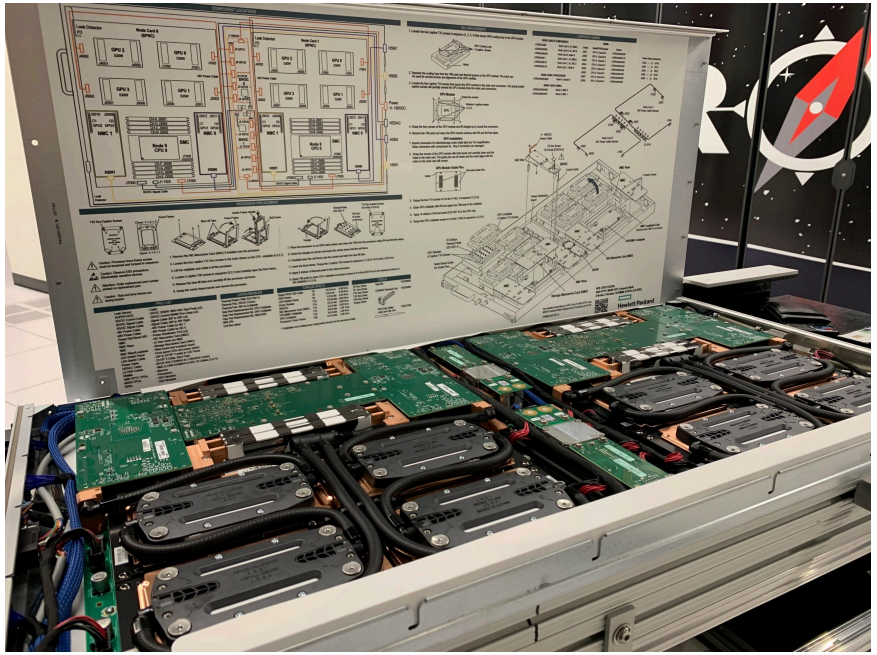
HPE Cray EX235A Blade

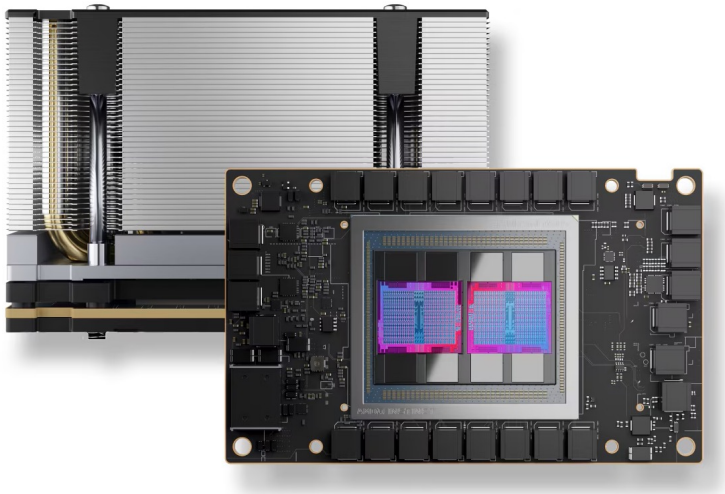
- 2x compute nodes per blade
  - Direct liquid cooled for all components
- Each node has:
  - 1x AMD Optimized 3rd Gen EPYC CPU
  - 4x AMD Instinct MI250X GPUs
  - 512 GB DDR4 on CPU
  - 512 GB HBM2e per node
  - 2x 1.92 TB NVMe, "Burst Buffer"
  - Full CPU & GPU connectivity with AMD Infinity Fabric
  - 4x HPE Slingshot 200 GbE NICs



https://www.hpcwire.com/wp-content/uploads/2022/06/ORNL-Frontier-blade-display-closer-June2022_4000x-scaled.jpg

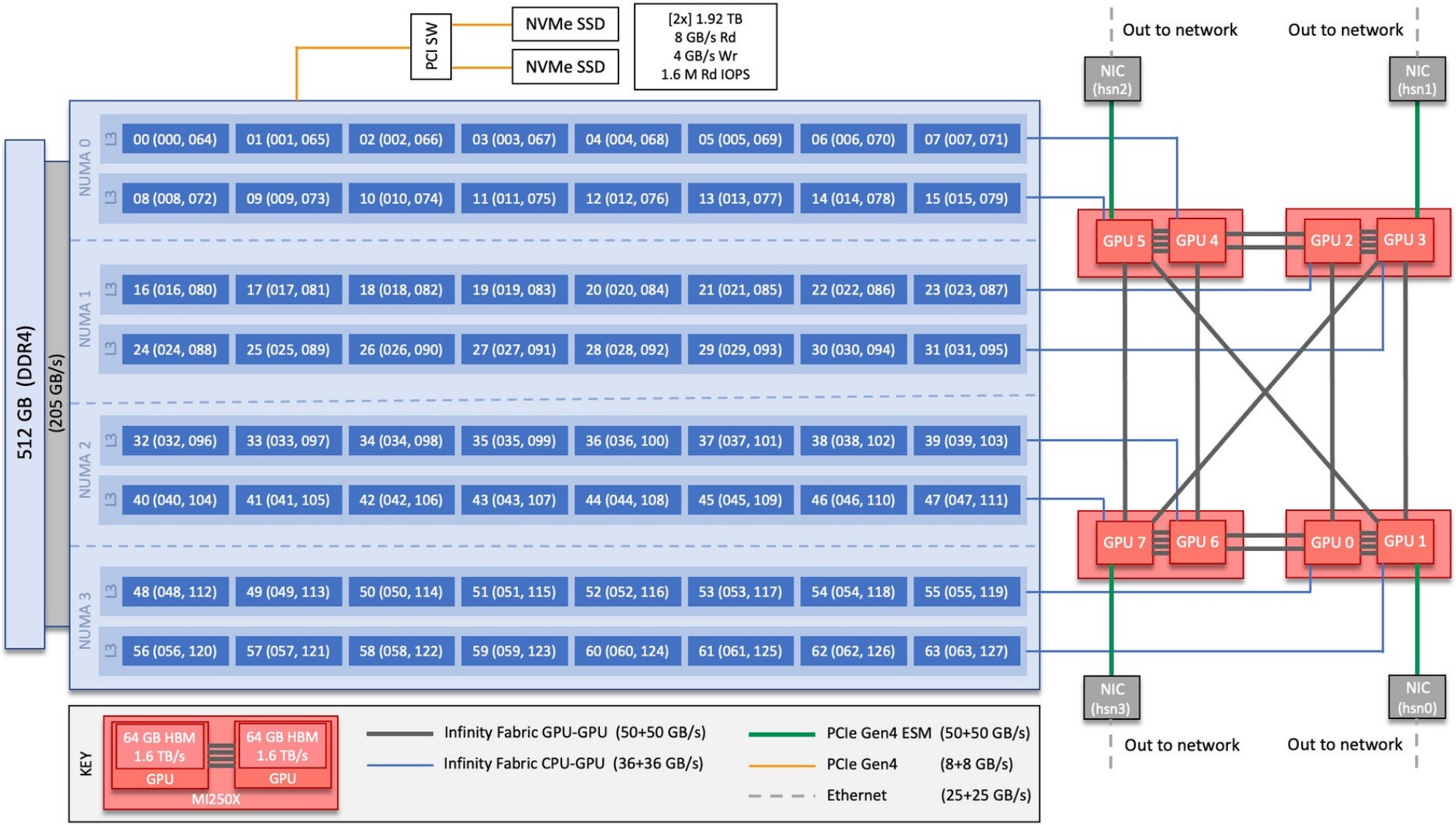
AMD Instinct MI250X GPU

- 2 Graphics Compute Dies (GCDs) per GPU
  - Shown by OS as 2 GPUs
- Effectively 8 GPUs per node, each with:
  - 110 Compute Units
  - 26.5 TFLOPs double-precision peak
  - 64 GB of HBM
  - 1.6 TB/s Memory Bandwidth
- Each associated with a CPU L3 cache region
- 1 NIC connected to each MI250X

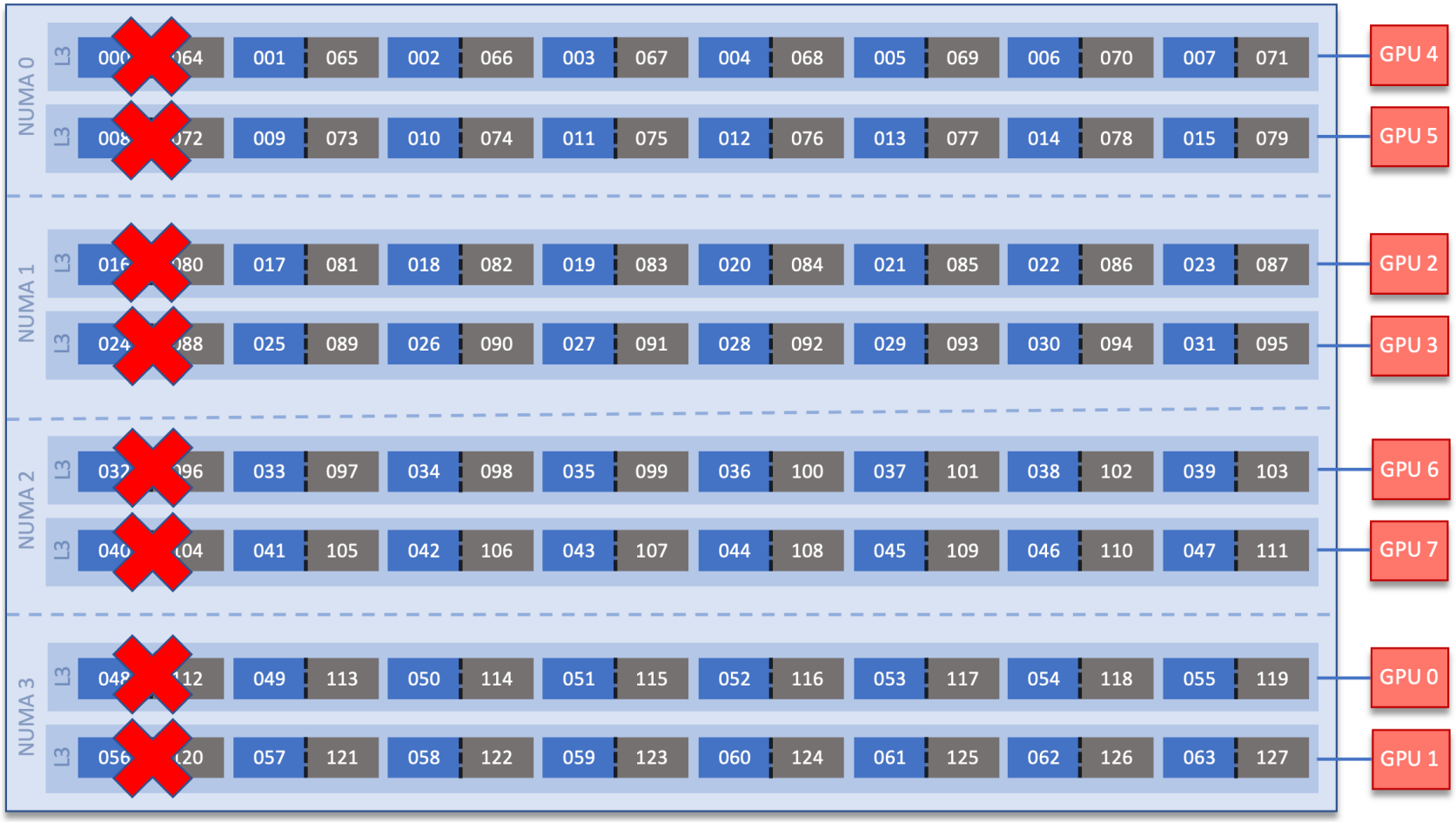


https://www.amd.com/content/dam/amd/en/images/products/data-centers/2325906-amd-instinct-mi250x-product.jpg

Frontier Node Diagram

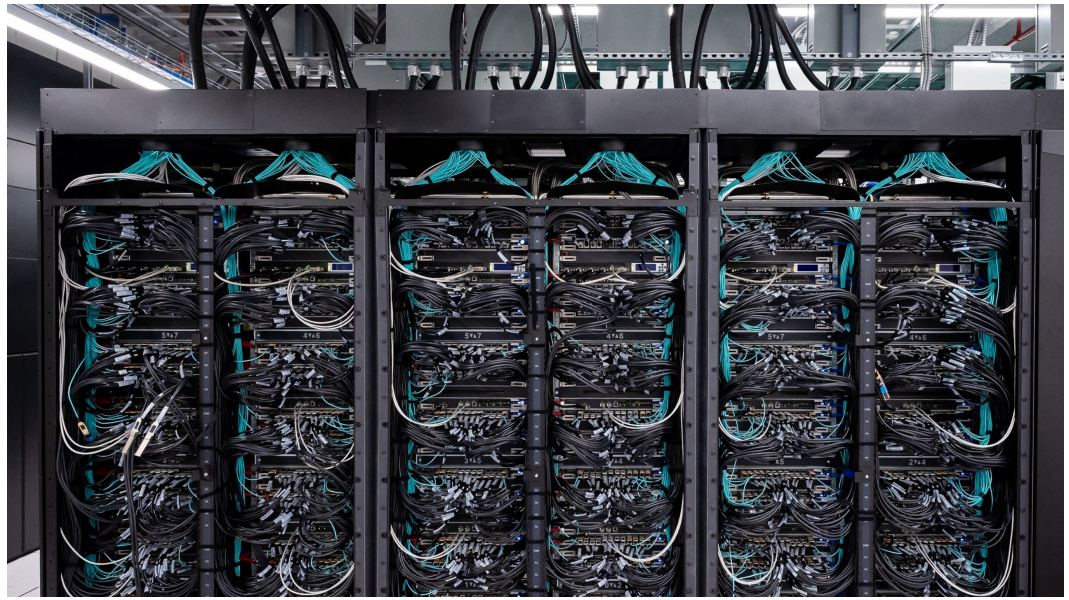


Frontier Node Diagram – Default Configuration



HPE Slingshot Interconnect

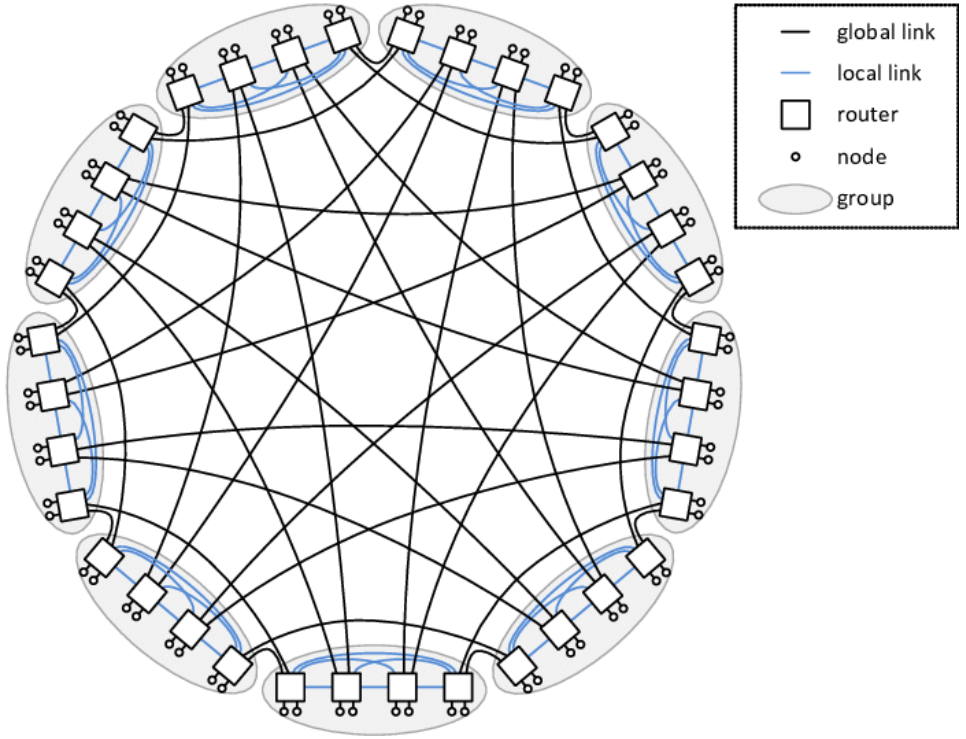
- High-speed, low latency network architecture
- HPE Slingshot switches (64 ports)
  - 25 GB/s bi-directional BW per port
- HPE Slingshot NICs
  - 25 GB/s bi-directional BW per link
- Slingshot is a superset of Ethernet with optimized HPC functionality
- Frontier uses dragonfly topology



https://www.ornl.gov/sites/default/files/2022-05/Side%20view%20Frontier%20cabinets.jpg

Frontier Network Topology

- Dragonfly groups
  - A group of endpoints connected to switches that are connected all-to-all
- Dragonfly topology
  - A set of groups connected all-to-all
    - Each group has >=1 link to every other group
- Frontier has 77 compute groups
  - 128 nodes per compute group
  - 32 switches per computer group
  - 4 NICs per node



https://www.researchgate.net/profile/Enrique-Vallejo-2/publication/261313973/figure/fig2/AS:667782257573894@1536223105142/Sample-Dragonfly-topology-with-h2-p2-a4-36-routers-and-72-compute-nodes.png

Frontier Programming Environment

- Compilers
  - Cray CCE
    - C/C++ LLVM-based
    - Cray Fortran
  - AMD ROCm
    - C/C++ LLVM-based
  - GCC
  - oneAPI DPC++
    - LLVM-based
    - user-managed

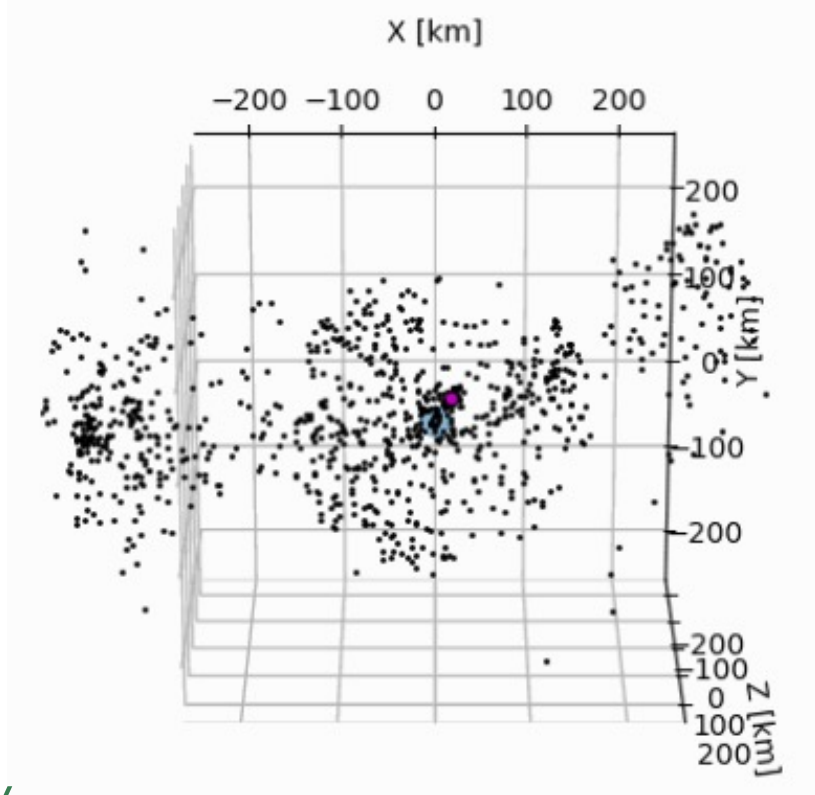
- Programming Models & Abstraction Layers
  - OpenMP
  - HIP
  - Kokkos
  - RAJA
  - SYCL
    - via user-managed DPC++
  - OpenACC
    - C/C++ via user-managed clacc
  - OpenCL
  - Julia
  - UPC++

OLCF System Access

- Odo available through TRN038
  - Odo is a 30-node Frontier training system
- System user guides:
  - https://docs.olcf.ornl.gov/systems/odo_user_guide.html
  - https://docs.olcf.ornl.gov/systems/frontier_user_guide.html
- Details on applying for an allocation of your own:
  - https://docs.olcf.ornl.gov/accounts/index.html
- Startup allocations with support also available:
  - https://www.olcf.ornl.gov/community/pathways-to-supercomputing/

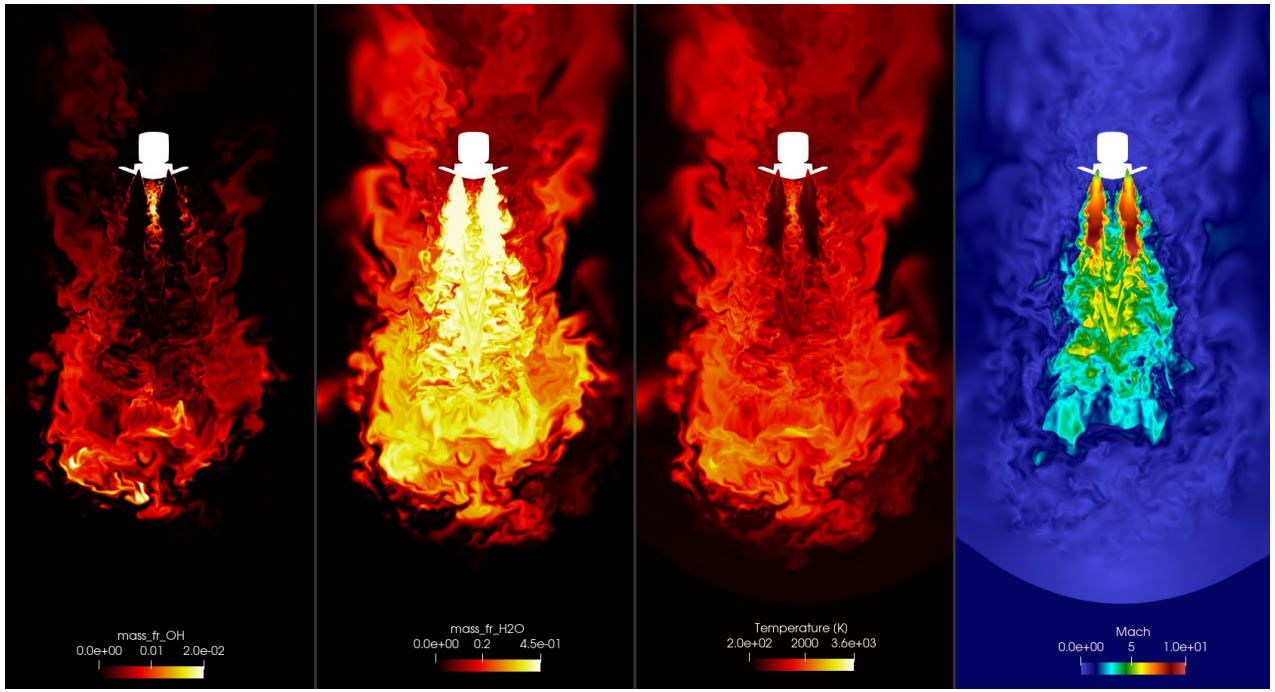
Hand-On Challenges

- Collection of self-guided challenges available to try:
  - https://github.com/olcf/hands-on-with-odo
- Challenges cover UNIX, programming environments, programming model basics, job schedulers, etc.
  - e.g., simulate and visualize galaxies colliding!
- OLCF support available in Slack
  - Additional support through help@olcf.ornl.gov



Example Frontier Use Case

- NASA is exploring ways to safely land a vehicle bringing humans to Mars
- Unable to flight-test in Martian environment
- Frontier enabled first-of-kind autonomous test flights
  - New levels of resolution, physical modeling, and temporal duration



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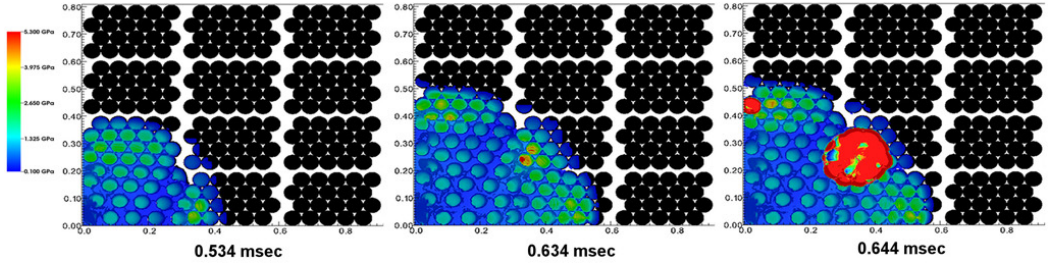
Example Leadership-Class Use Case

- Semi hauling 35,000 pounds of mining explosives crashed in Utah
- Caught fire and caused dramatic explosion leaving a 30'x70' crater
- Debris launched up to 1/4 mile
- Leadership-class systems (e.g., Titan) used to recreate explosion
- Simulations helped identify safer ways to pack mining explosives

https://www.summitdaily.com/news/trailer-full-of-explosives-blows-hole-in-utah/



https://www.jics.tennessee.edu/files/images/accidental-explosion1.jpg

Fun Facts

- 1 Exaflop => 10^{18} Calculations per Second
  - Frontier can do in 1 second what'd take over 4 years if everyone on Earth did 1 calculation/s
- 2.1 Exaflop peak double-precision
  - Compute similar to ~204K PS5s
- 77 cabinets weighing 8,000 pounds each
  - Total weight similar to a Boeing 747
- 700 PB of storage
  - 25 Mt. Everests of DVDs

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OAK RIDGE National Laboratory

Questions?

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