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Ready for Aurora

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26 March 2025

Abstract

The webinar will highlight the wide variety of applications that are ready to run on Aurora's PVC GPU-accelerated architecture. In addition to representing many different scientific domains, the project workflows include many numerical methods, AI models for training and inference loads, and a variety of programming approaches for the PVC GPUs.

Aurora

Intel® Data Center GPU Max Series

4th Gen Intel XEON Max Series CPU *with High Bandwidth Memory*

Platform
HPE Cray-Ex

Racks - 166
Nodes - 10,624
   CPUs - 21,248
   GPUs – 63,744

Interconnect
HPE Slingshot 11
Dragonfly topology with adaptive routing
Cassini NIC, 200 Gb/s (25 GB/s), 8 per node
Network Switch:
   25.6 Tb/s per switch (64 200 Gb/s ports)
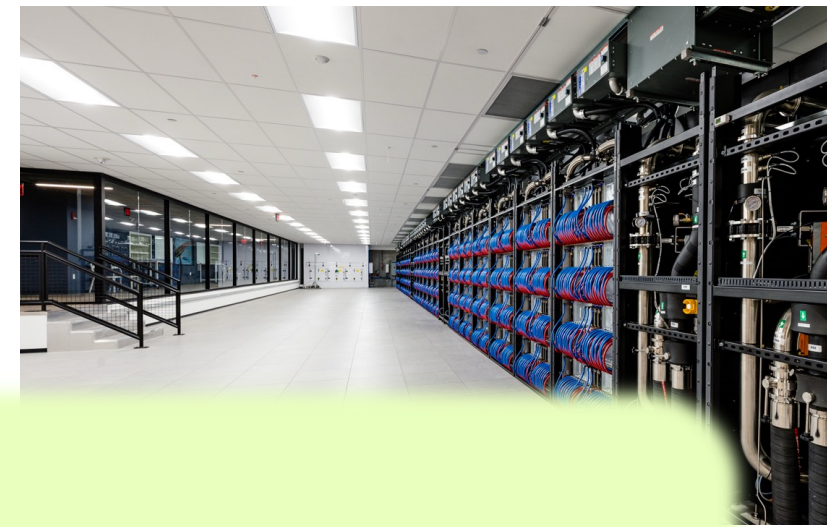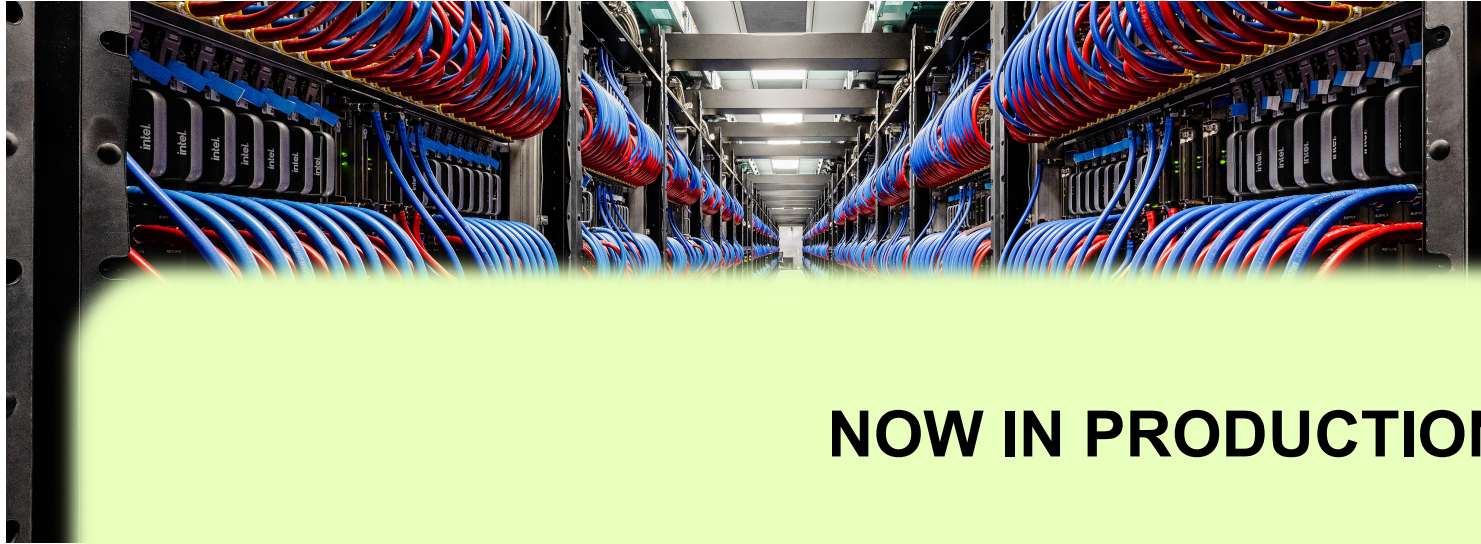   Links with 25 GB/s per direction

Peak FP64 Performance
$\geqq$ **2 exaFLOPS**

Memory
10.9PiB of DDR @ 5.95 PB/s
1.36PiB of CPU HBM @ 30.5 PB/s
8.16PiB of GPU HBM @ 208.9 PB/s

Network
2.12 PB/s Peak Injection BW
0.69 PB/s Peak Bisection BW

Storage
230PB DAOS Capacity
31 TB/s DAOS Bandwidth

Aurora

NOW IN PRODUCTION!

#3 in Top500 w/9234 nodes – HPL 1.012 exaFLOPS

#1 in Top500 w/9500 nodes – HPL-MxP 11.6 exaFLOPS

Int...
Ma...

4th
Se...
Ban...

Dragonfly topology with adaptive routing
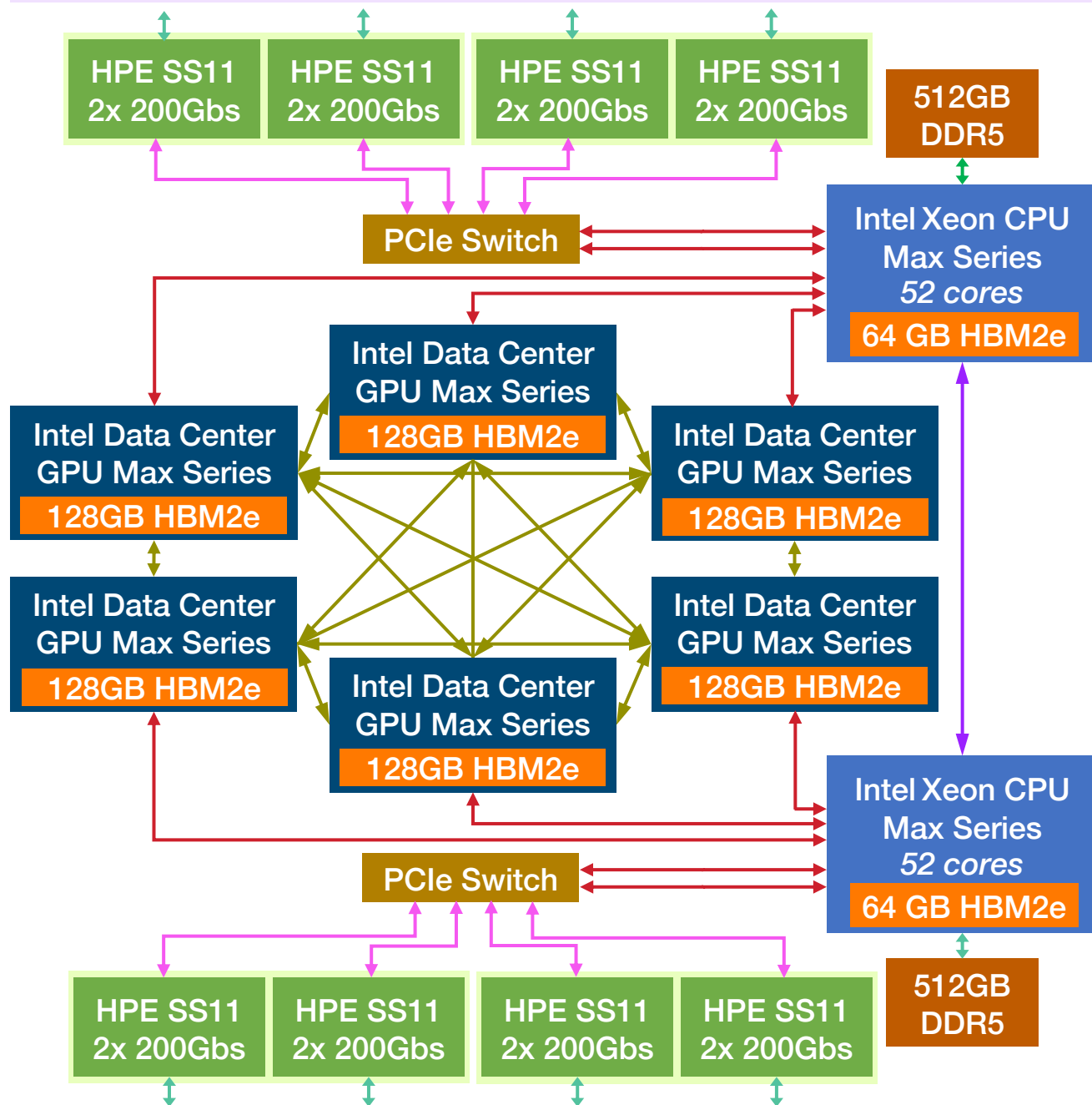Cassini NIC, 200 Gb/s (25 GB/s), 8 per node
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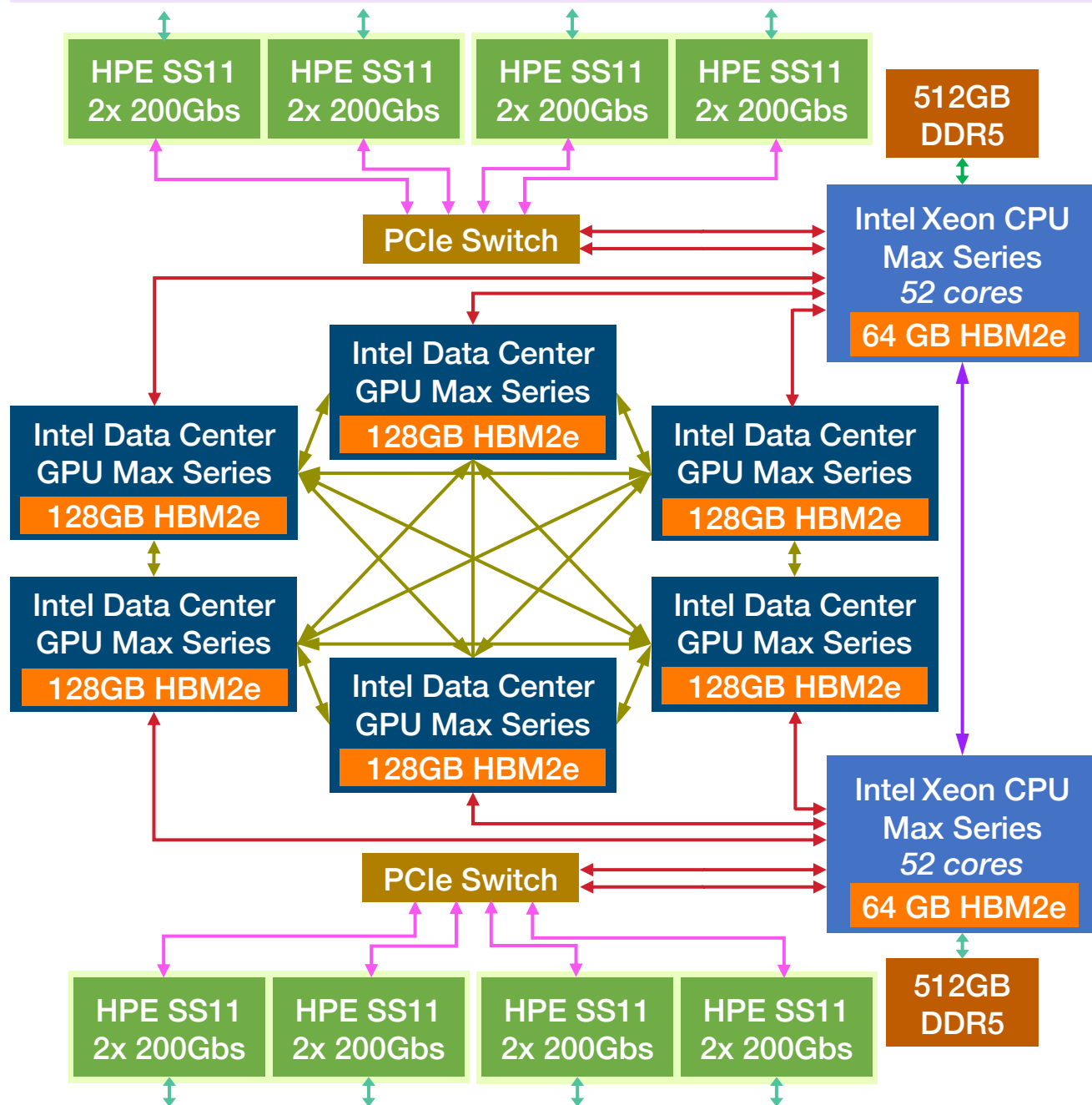
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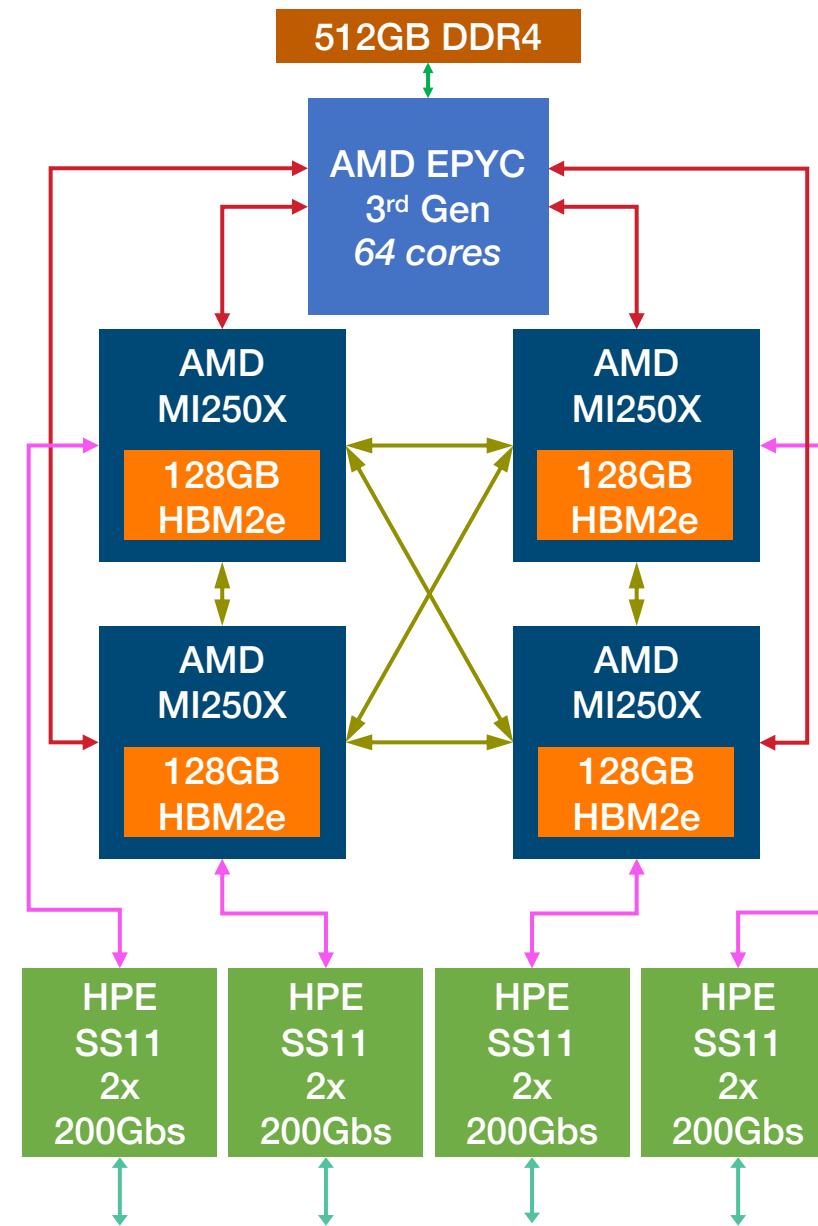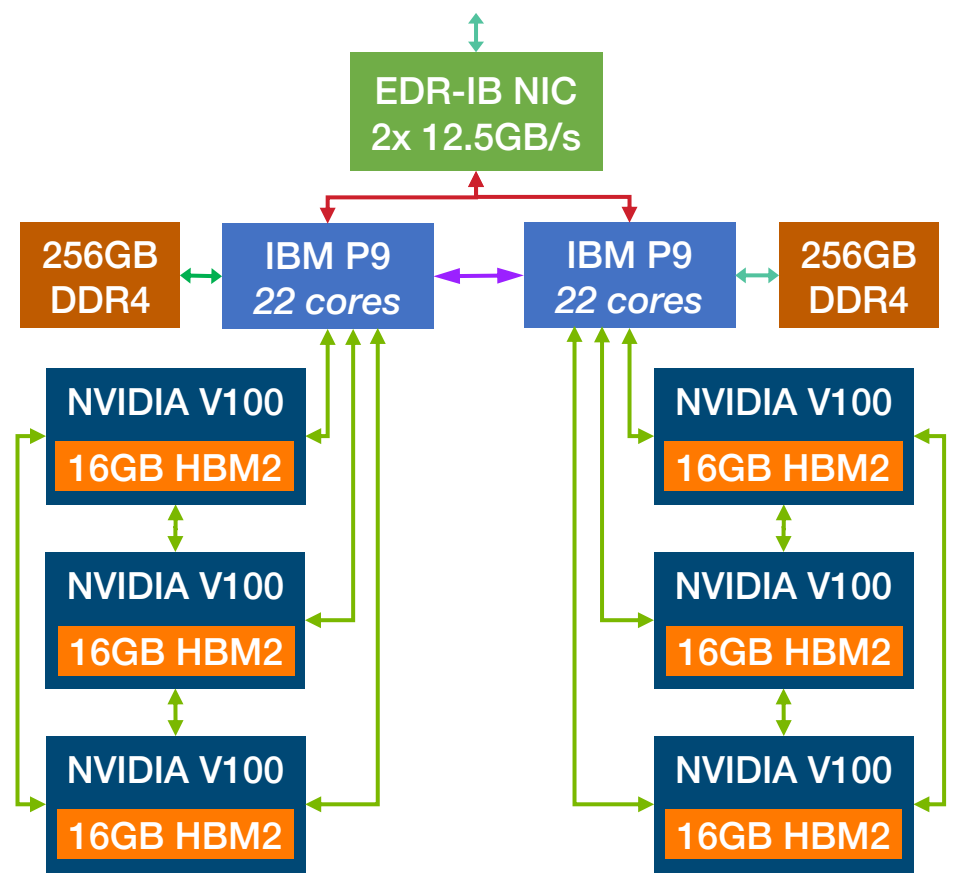
Storage
230PB DAOS Capacity
31 TB/s DAOS Bandwidth

Platform
HPE Cray-Ex

Aurora Node

| HPE SS11 2x 200Gbs | HPE SS11 2x 200Gbs | HPE SS11 2x 200Gbs | HPE SS11 2x 200Gbs | 512GB DDR5 |

PCIe Switch

Intel Xeon CPU Max Series *52 cores* — 64 GB HBM2e

Intel Data Center GPU Max Series — 128GB HBM2e

Intel Data Center GPU Max Series — 128GB HBM2e

Intel Data Center GPU Max Series — 128GB HBM2e

Intel Data Center GPU Max Series — 128GB HBM2e

Intel Data Center GPU Max Series — 128GB HBM2e

Intel Data Center GPU Max Series — 128GB HBM2e

Intel Xeon CPU Max Series *52 cores* — 64 GB HBM2e

PCIe Switch

| HPE SS11 2x 200Gbs | HPE SS11 2x 200Gbs | HPE SS11 2x 200Gbs | HPE SS11 2x 200Gbs | 512GB DDR5 |

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Pre-Exascale Systems

Pre-Exascale Systems

Polaris at ALCF

Summit at OLCF

HPE SS11 2x 200Gbs	HPE SS11 2x 200Gbs

NVIDIA GPUs

EDR-IB NIC 2x 12.5GB/s

512G

256GB DDR4

256GB DDR4

AMD Milan *32 cores*

IBM P9 *22 cores*

IBM P9 *22 cores*

NVIDIA A100 40GB HBM2

NVIDIA A100 40GB HBM2

NVIDIA A100 40GB HBM2

NVIDIA A100 40GB HBM2

NVIDIA V100 16GB HBM2

NVIDIA V100 16GB HBM2

NVIDIA V100 16GB HBM2

NVIDIA V100 16GB HBM2

NVIDIA V100 16GB HBM2

NVIDIA V100 16GB HBM2

Aurora Applications/Software Readiness Efforts

- Exascale Computing Project (ECP) 2016-2023
  - 7 years, $1.8B, 2800 people
    - 15 (of 21) Applications Development projects engaged with ALCF toward Aurora
    - ALCF POC for each, via ECP Hardware & Integration funding

- Aurora Early Science Program (ESP)
  - 19 project teams with over 200 multi-institutional team members
    - 16 ALCF postdocs
    - 19 ALCF Catalysts/POCs (10% effort for ~7 years)

- Intel-Argonne Center of Excellence
  - 5 Intel staff
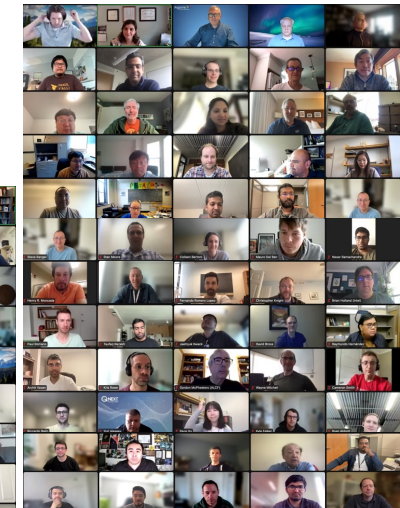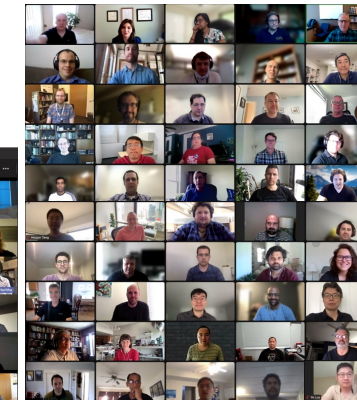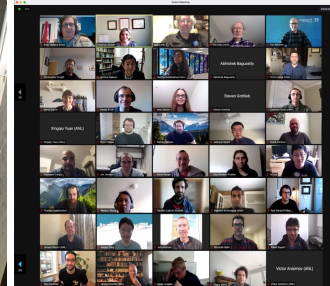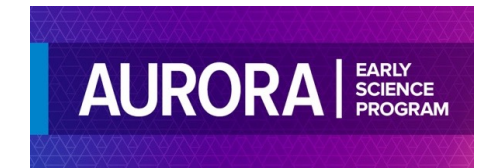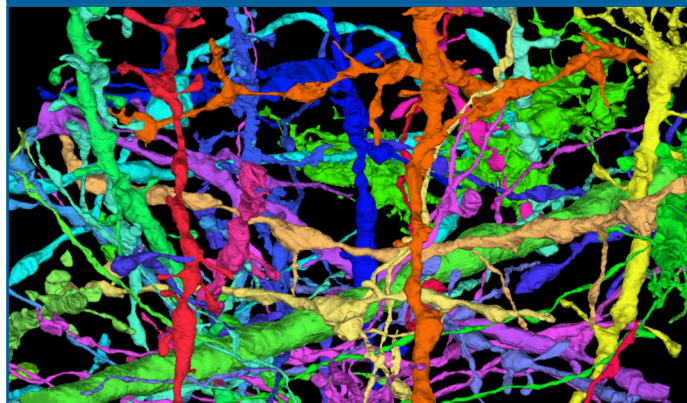
Aurora Early Science Program

Science campaigns start 1/27 with workflows incorporating the 3 pillars

Simulation
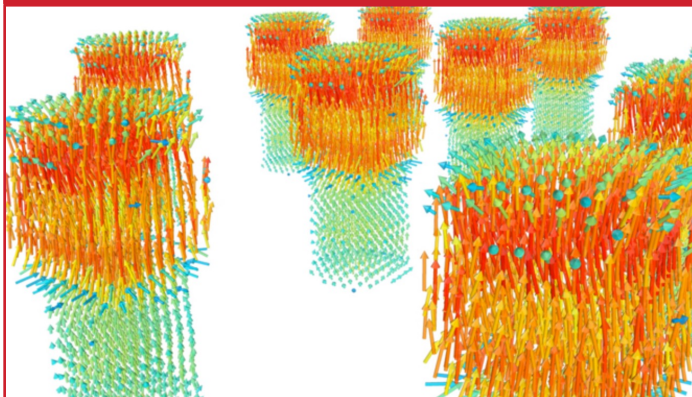
- Reactive, quantum, and classical MD for materials and biophysics
- ITER tungsten impurity ions kinetics—PIC
- Cosmological P^3M + SPH hydrodynamics
- CCSD(T) quantum chemistry
- Quantum Monte Carlo
- FEM CFD, CFD+combustion

Data

- High-throughput electron microscopy data
- In situ data from blood flow and aerodynamics simulation
- Atlas detector event Monte Carlo analysis
- Cosmological sky survey and P^3M simulation data
- Chemistry kinetics database
- Tokamak experiment data

Learning
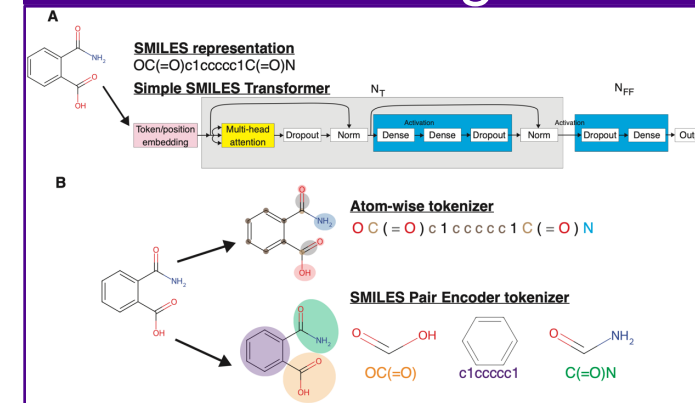
- Simple SMILES transformer for drug design
- Generative model for lattice QCD
- Material band gap predictor
- Tokamak disruption predictor
- Flood fill model for connectomics
- MLP turbulence closure model

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First-Year Science Projects on Aurora

ALCF Node-Hours

- ■ Aurora Early Science Program (ESP)
  - – 19 projects
  - – 19.8 million node-hours

- ■ INCITE
  - – 30 projects (+ 4 porting/optimization projects)
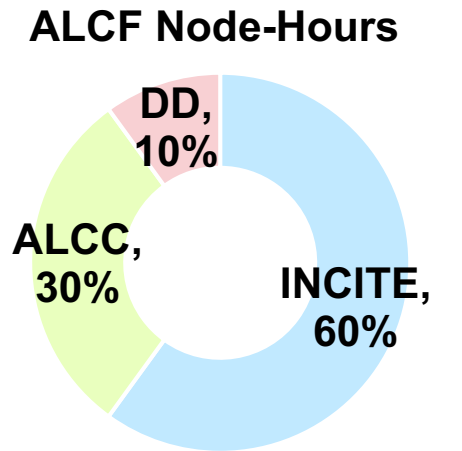 - – 22.6 million node-hours

Open to researchers from academia, government laboratories, and industry, the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program is the major means by which the scientific community gains access to the nation's fastest supercomputers. The program aims to accelerate scientific discoveries and technological innovations by awarding, on a competitive basis, time on supercomputers to researchers with large-scale, computationally intensive projects that address "grand challenges" in science and engineering.

- ■ ALCC (ASCR Leadership Computing challenge)
  - – 13 projects
  - – 5 million node-hours

Computational Science Methods in Y1 Aurora Projects

Molecular Dynamics
- classical
- reactive
- quantum
- multiscale
- NN force fields

Particle Methods
- Monte Carlo transport
- P³M
- plasma PIC

AI
- federated learning
- protein folding
- flow-based generative model
- CNN
- RNN
- FFN
- LLM (GPT)
- SST
- gaussian process
- equivariant NN
- hyperparameter tuning

Lattice QCD
Quantum Circuit Simulation
Nuclear QMC

Quantum Chemistry
- coupled cluster
- QMC
- HF
- EFMO
- DFT
- RI-MP2
- plane-wave DFT
- GW

CFD
- LBM
- finite element
- combustion
- finite volume
- spectral element
- DNS, LES, WMLES
- AMR
- SPH
- GR-MHD

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Computational Science Methods in Y1 Aurora Projects + ECP

Molecular Dynamics
- classical
- reactive
- quantum
- multiscale
- NN force fields

Particle Methods
- CFD PIC
- Monte Carlo transport
- P³M
- PM
- plasma PIC

direct kinetic solver

**Lattice QCD
Quantum Circuit Simulation
Nuclear QMC**

AI
- federated learning
- protein folding
- flow-based generative model
- CNN
- RNN
- FFN
- SST
- gaussian process
- LLM (GPT)
- equivariant NN
- hyperparameter tuning

Quantum Chemistry
- coupled cluster
- QMC
- HF
- EFMO
- DFT
- RI-MP2
- plane-wave DFT
- GW

CFD
- super-parameterization
- finite element
- combustion
- finite difference
- spectral element
- finite volume
- MOL
- CFD-DEM
- GR-MHD
- DNS, LES, WMLES
- AMR
- PPM

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Science Domains in Y1 Aurora Projects

Aerodynamics
Combustion
Thermal hydraulics for fusion & fission
Turbulent Rayleigh-Benard convection
Buoyancy-driven turbulence
Wind energy

Fusion radiation transport
Fusion plasma kinetics
Tokamak control

Neuroscience foundation model
Science foundation model
Federated learning
Quantum computing
AI assistant for simulation

Core collapse supernovae
Binary neutron star mergers
Core collapse supernovae
Black hole accretion
Neutron star remnants

Functional quantum materials
Fusion device materials
Multiscale materials modeling
Quantum materials
Materials science

QCD
Cosmology
Nuclear structure and reactions
Collider data analysis

MOF design
Carbon capture
Transition metal chemistry
Heterogeneous catalysis
Heterogeneous reactions
Biofuels

Membrane transport proteins
Predictive molecular epdimiology
Blood flow & transport
Cancer drug design
Heteropolymer design
Brain connectomics
Pathogenesis

Climate modeling
Runoff inundation

Science Domains in Y1 Aurora Projects + ECP

Aerodynamics Combustion

Thermal hydraulics for fusion & fission

Turbulent Rayleigh-Benard convection

Buoyancy-driven turbulence

Wind energy

Fusion radiation transport

Fusion plasma kinetics

Tokamak control

Neuroscience foundation model

Science foundation model

Federated learning Quantum computing

AI assistant for simulation

Core collapse supernovae

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Neutron star remnants

Functional quantum materials

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Multiscale materials modeling

Quantum materials Materials science

QCD Cosmology

Nuclear structure and reactions

Collider data analysis

MOF design Carbon capture

Transition metal chemistry

Heterogeneous catalysis

Heterogeneous reactions Biofuels

Membrane transport proteins

Predictive molecular epdimiology

Blood flow & transport

Cancer drug design

Heteropolymer design

Brain connectomics

Pathogenesis

Climate modeling

Runoff inundation

Seismic wave propagation

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Aurora Y1 and ECP Applications by Name

| INCITE, ALCC, ESP, ECP Applications With PVC Offload			
AMR-Wind	DiffLinker	HARVEY	QUDA
Allegro	E3SM-MMF	HemeLB_GPU	Quantum Espresso
Alphafold2	ExaChem	LAMMPS	RXMD-NN
AthenaK	FLARE	MFDn	Rosetta
AuroraGPT	FUN3D	MFIX-Exa	SCREAM
BerkeleyGW	FastCaloSim	MILC	SR-APPFL
CANDLE/Uno	Flood Fill Network	MadGraph	SST
CEED-PHASTA	Fornax	Masala	SwiFT
CHROMATIX	FusionDL	NAMD	TRITON
CP2K	GAMESS	NWChemEx	Thornado/Flash-X
CPS	GENE	NekRS	UIntah
Chroma	GTC	OpenMC	Uno
Contegra	GURU	OpenMM	XGC
DCMESH	Grid	PHASTA	
DarkSkyML	H-AMR	PWDFT	
DataDrivenCFD	HACC	QMCPACK	

Aurora Performance and Expectations

- DOE Exascale Computing Project (ECP)
  - Achieve 50X improvement in figure-of-merit (FOM) w.r.t. pre-ECP baseline (2017 systems)
  - Aurora: 3 projects measured this:
    - EXAALT – 89X on 1024 nodes
    - ExaSMR – 84X on 512 nodes
    - ExaSky – 277X on 4096 nodes

- Aurora Early Science Program (ESP)
  - Demonstrate INCITE-level computational readiness
    1. Scale efficiently to 20% of full system
    2. Make use of GPUs
    3. Ready to run science in 1-3 months
 - Internal+external review: 16/19 projects met goal in Fall 2024
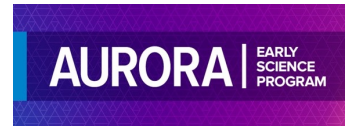
Aurora Performance and Expectations

- Argonne Applications Working Group performance tracked single-GPU performance figures of merit across >25 ECP and ESP applications for several years
  - Expectations
    - Comparable performance to AMD MI-250X (Frontier GPU)
    - Better performance than NVIDIA A100 (Polaris GPU)

PVC/MI250X Performance Ratio

PVC/A100 Performance Ratio
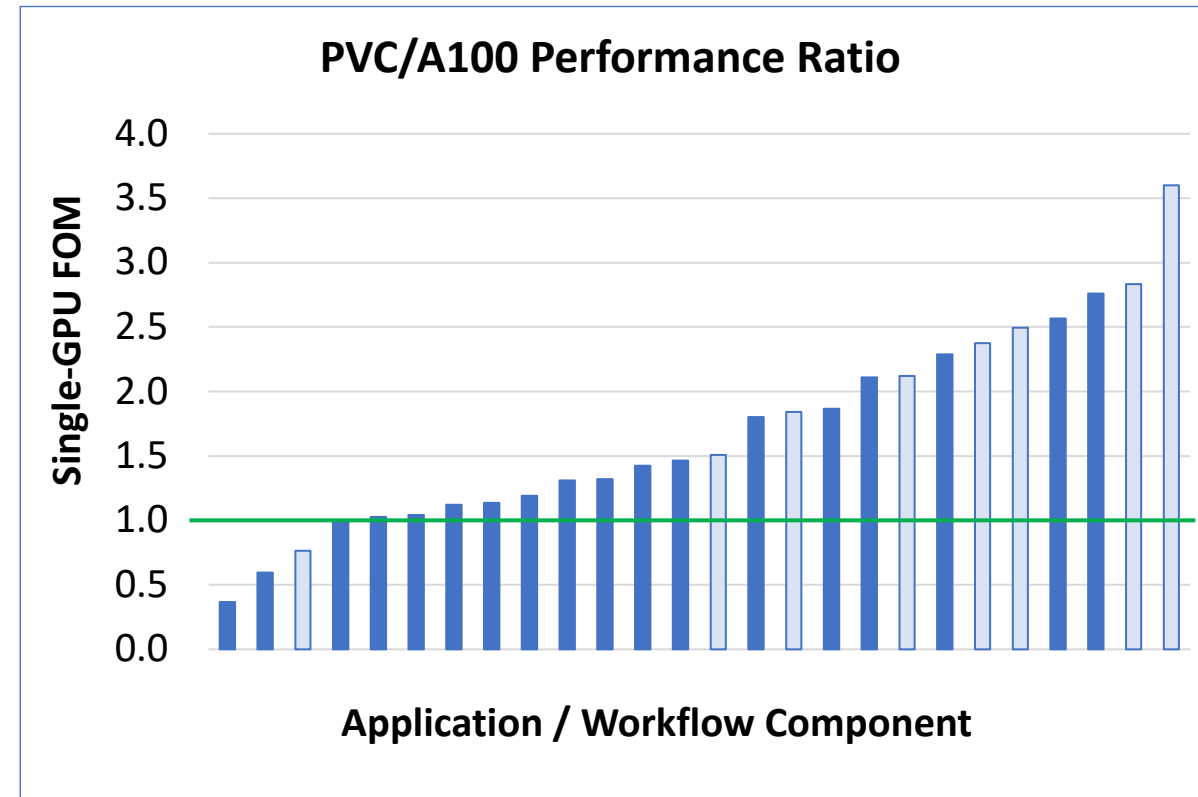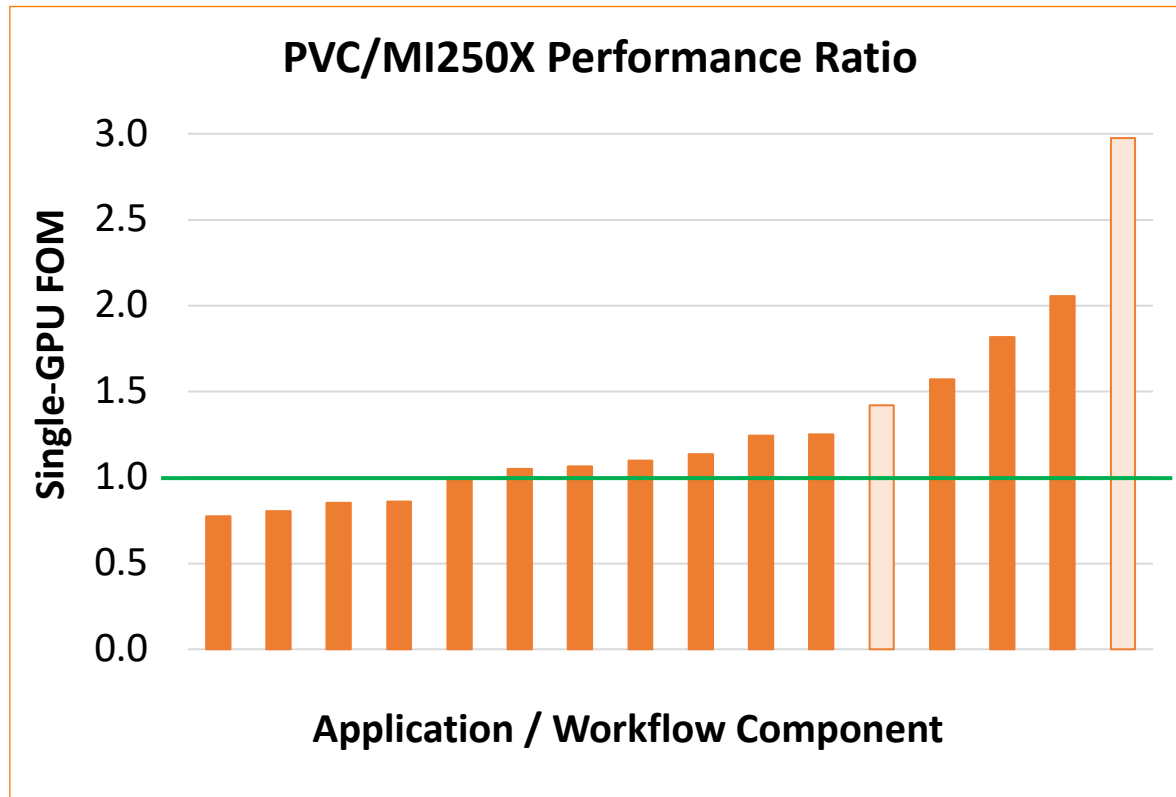
Exascale Programming Models – Data & Learning
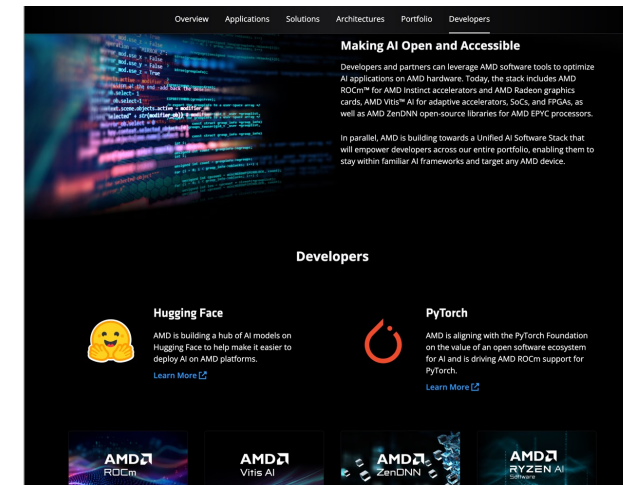
- AI / data science community expects portability via Python ecosystem
  - Python – Numba, NumPy, etc.
  - Deep learning frameworks
    - PyTorch, TensorFlow, JAX, DeepSpeed, Horovod
- Hardware vendors optimize performance (NVIDIA, Intel, AMD)
  - GPU offload
  - communication for distributed training & inference
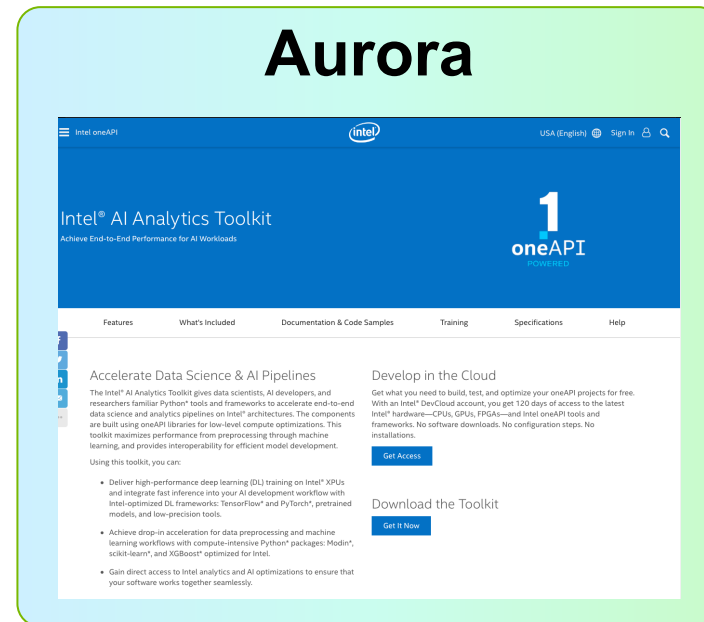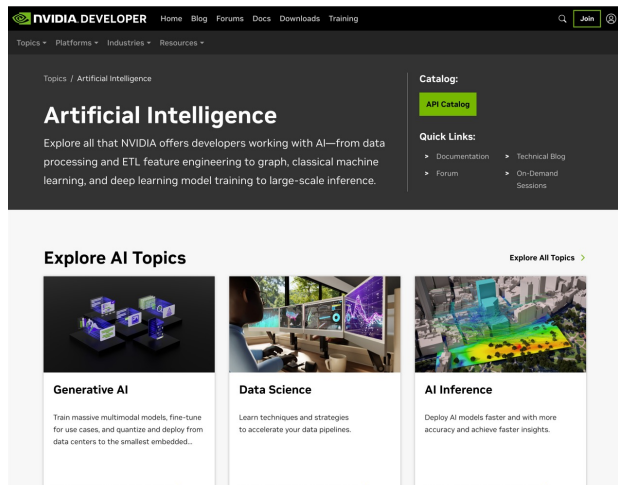
Aurora

https://docs.alcf.anl.gov/aurora/data-science/python/

Exascale Programming Models – Simulation

- CPU: portability via OpenMP threads and SIMD

- Communication: portability via MPI

- GPU: portability via OpenMP `target`

- GPU: other offload kernel programming:

NVIDIA	Intel	AMD
CUDA	CUDA (chipStar, Syclomatic)	CUDA (HIPIFY)
HIP	HIP (chipStar)	**HIP**
SYCL	**SYCL**	SYCL
OpenCL	OpenCL	OpenCL

Portability layers/libraries

- Kokkos, Raja, libCEED, OCCA, AMReX, PETSc
- DIY

CUDA	SYCL	HIP

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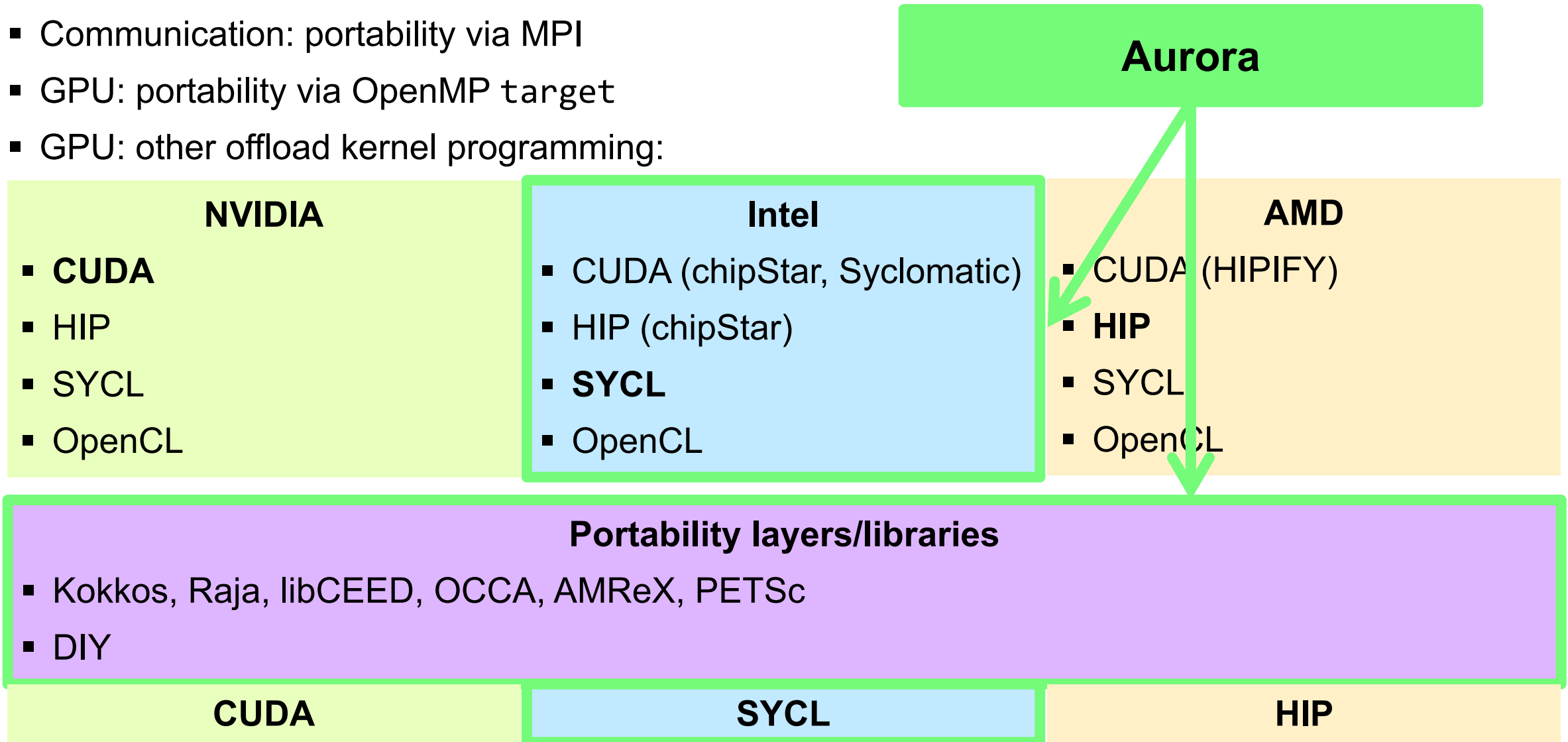NATIONAL LABORATORY

Exascale Programming Models – Simulation

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NVIDIA	**Intel**	**AMD**
CUDA	CUDA (chipStar, Syclomatic)	CUDA (HIPIFY)
HIP	HIP (chipStar)	**HIP**
SYCL	**SYCL**	SYCL
OpenCL	OpenCL	OpenCL

Portability layers/libraries

- Kokkos, Raja, libCEED, OCCA, AMReX, PETSc

- DIY

CUDA	**SYCL**	**HIP**

Programming Model Choices by Y1 Aurora Projects

Project Counts

- Kokkos-kernels, 1
- OpenCL, 1
- PETSc, 3
- HIP, 2
- OCCA, 5
- libCEED, 3
- Grid, 4
- QUDA, 4
- AI Frameworks, 19
- Kokkos, 13
- SYCL, 19
- OpenMP, 16

Programming Model Choices by Y1 Aurora Projects **+ ECP**

Pie chart titled "Project Counts" showing programming model choices:
- OpenMP, 22
- SYCL, 23
- Kokkos, 17
- AI Frameworks, 20
- QUDA, 5
- Grid, 5
- libCEED, 3
- OCCA, 6
- HIP, 3
- PETSc, 3
- Kokkos-kernels, 1
- OpenCL, 1
- Raja, 1