

# Exascale Science on Aurora

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2023-10-21

# About Me

-  [samforeman.me](http://samforeman.me)
    - [Data Science @ ALCF](#)
  - Undergrad (2010 — 2015):
    - UIUC:
      - Engineering Physics
      - Applied Mathematics
  - Grad School (2015 — 2019):
    - University of Iowa
      - PhD. Physics
      - ["A Machine Learning Approach to Lattice Gauge Theory"](#)
  - Postdoc (2019-2022) @ ALCF
- **Current Research:**
    - [AI + Science:](#)
      - [\*GenSLMs: Genome-scale language models reveal SARS-CoV-2 evolutionary dynamics\\*\*](#)
      - [Building better sampling methods for Lattice QCD](#)
      - [Foundation models for long term climate forecasting](#)
    - [Scaling Large Language Models](#)
      - [Optimizing distributed training across thousands of GPUs](#)
      - Building new parallelism techniques for efficient scaling
    - You can get a live view of some of my recent talks [here](#)

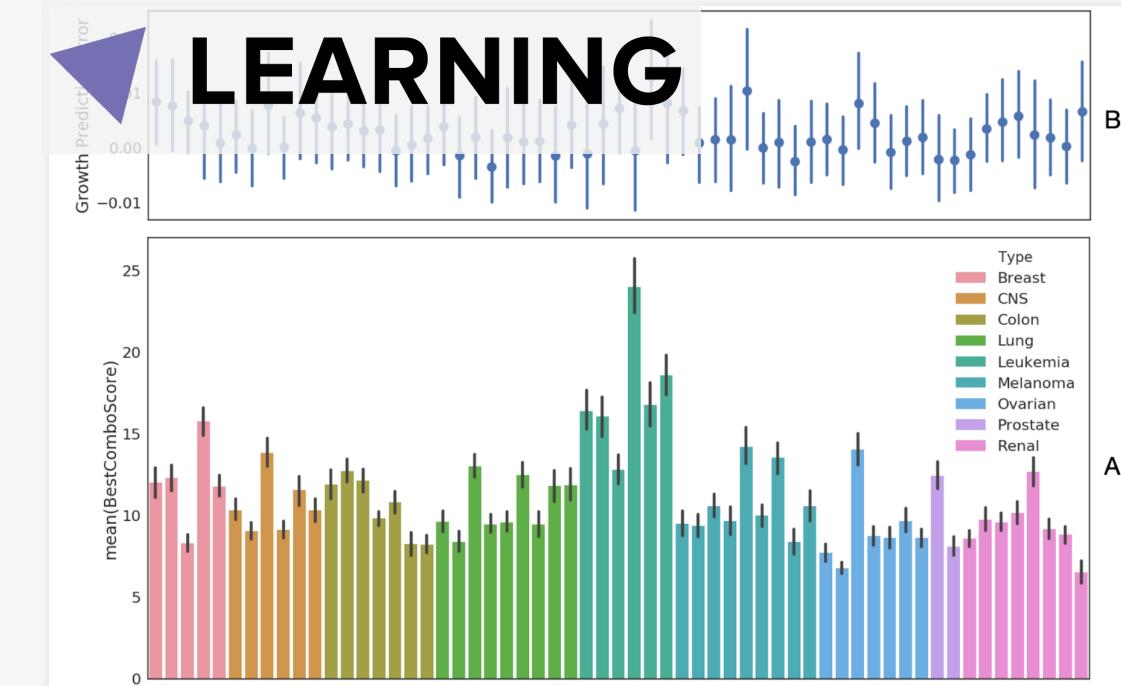
\*[ACM Gordon Bell Special Prize for HPC-Based COVID-19 Research](#)

# Argonne Leadership Computing Facility (ALCF)

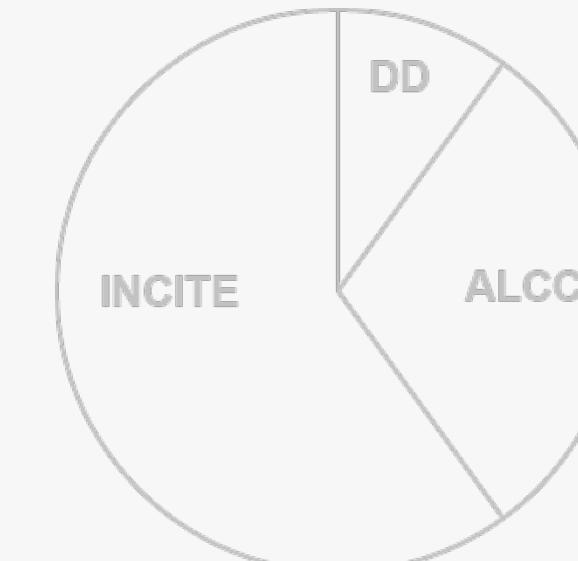


The [ALCF](#) provides world-class computing resources to the scientific community.

- Users pursue scientific challenges
- In-house experts help maximize results
- Resources **fully dedicated to open science**



**ALCF offers different pipelines based on your computational readiness.**



(Apply to the allocation program that fits your needs)



Architecture supports three types of computing:

- 1. Large-scale Simulation**
  - PDEs, traditional HPC
- 2. Data Intensive Applications**
- 3. Deep Learning and Emerging Science AI**

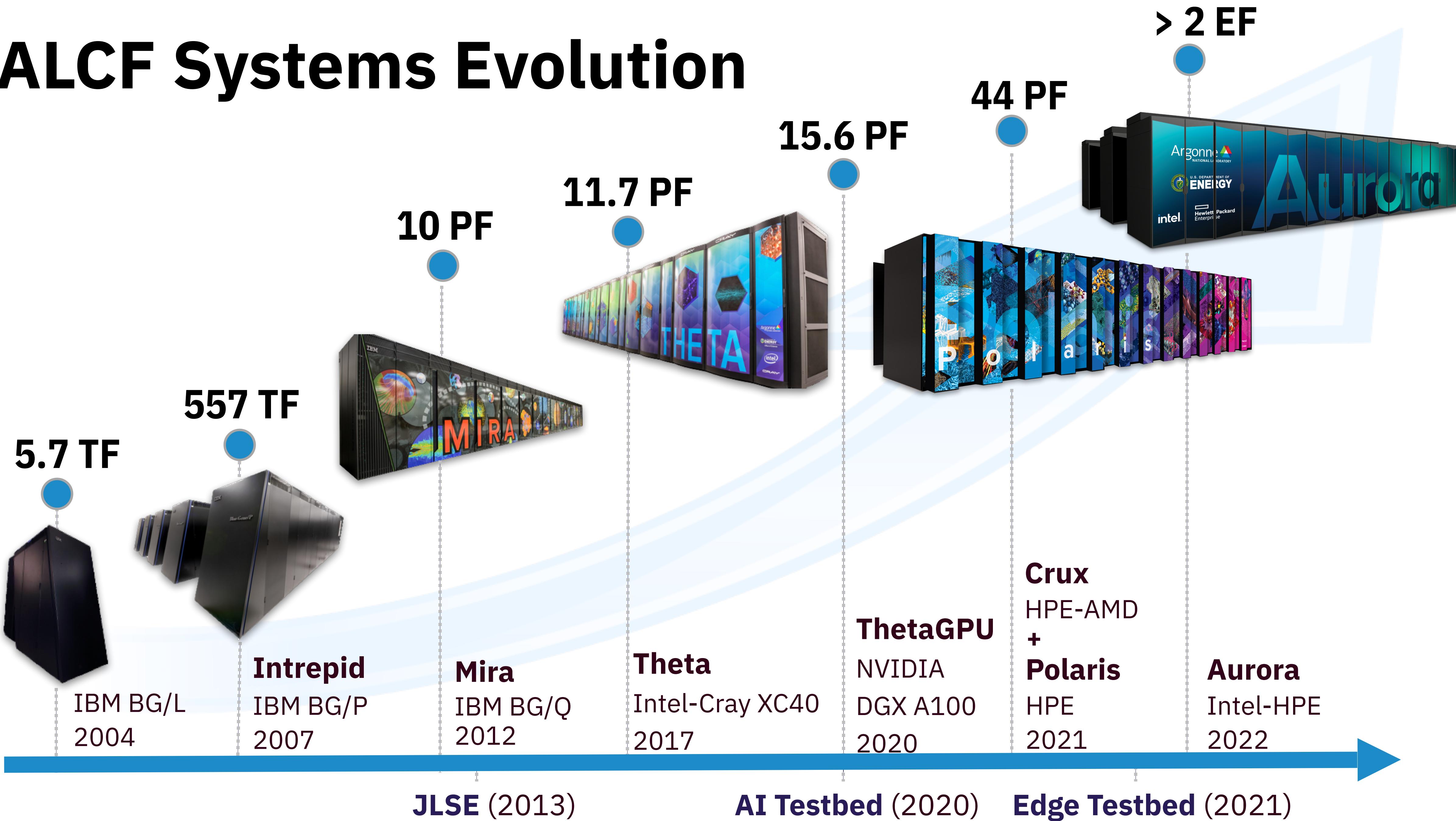
- Training + inference
- Scalable pipelines

# ALCF



Full Group @ ALCF (+ summer students !!)

# ALCF Systems Evolution

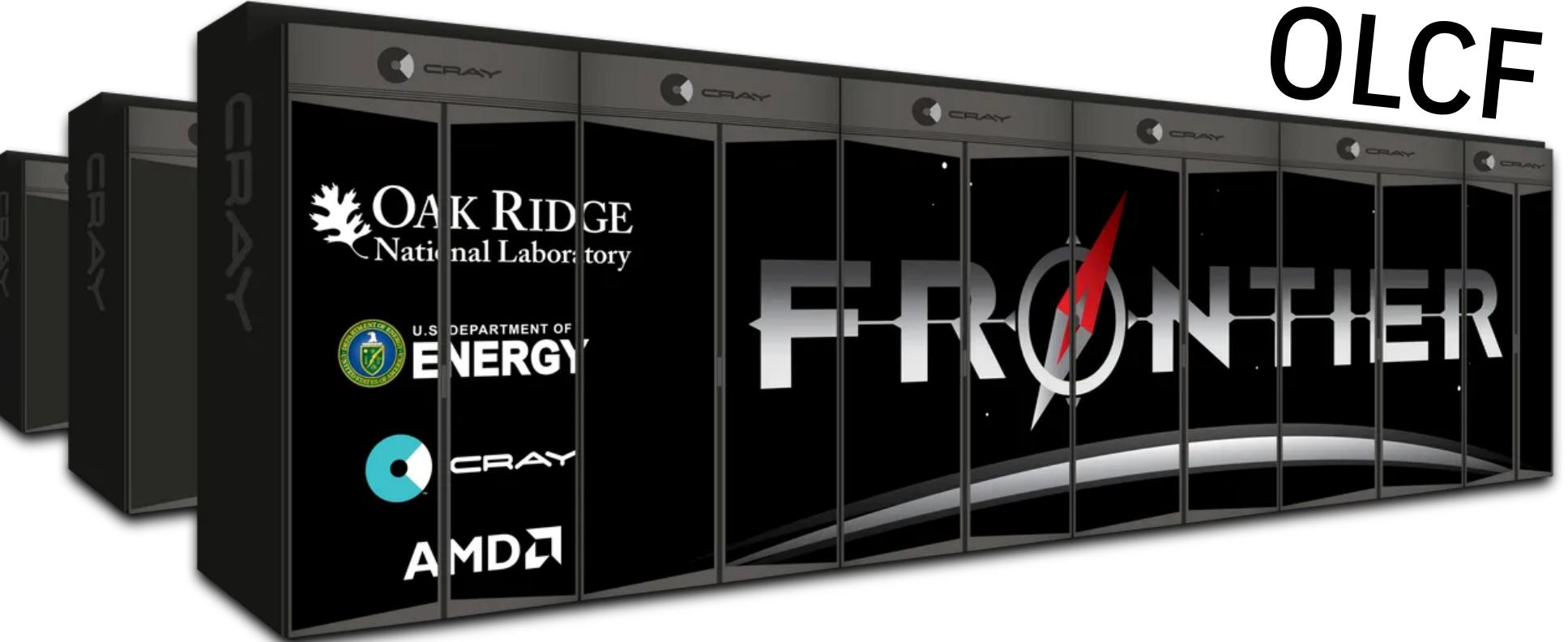


# US Exascale Platforms

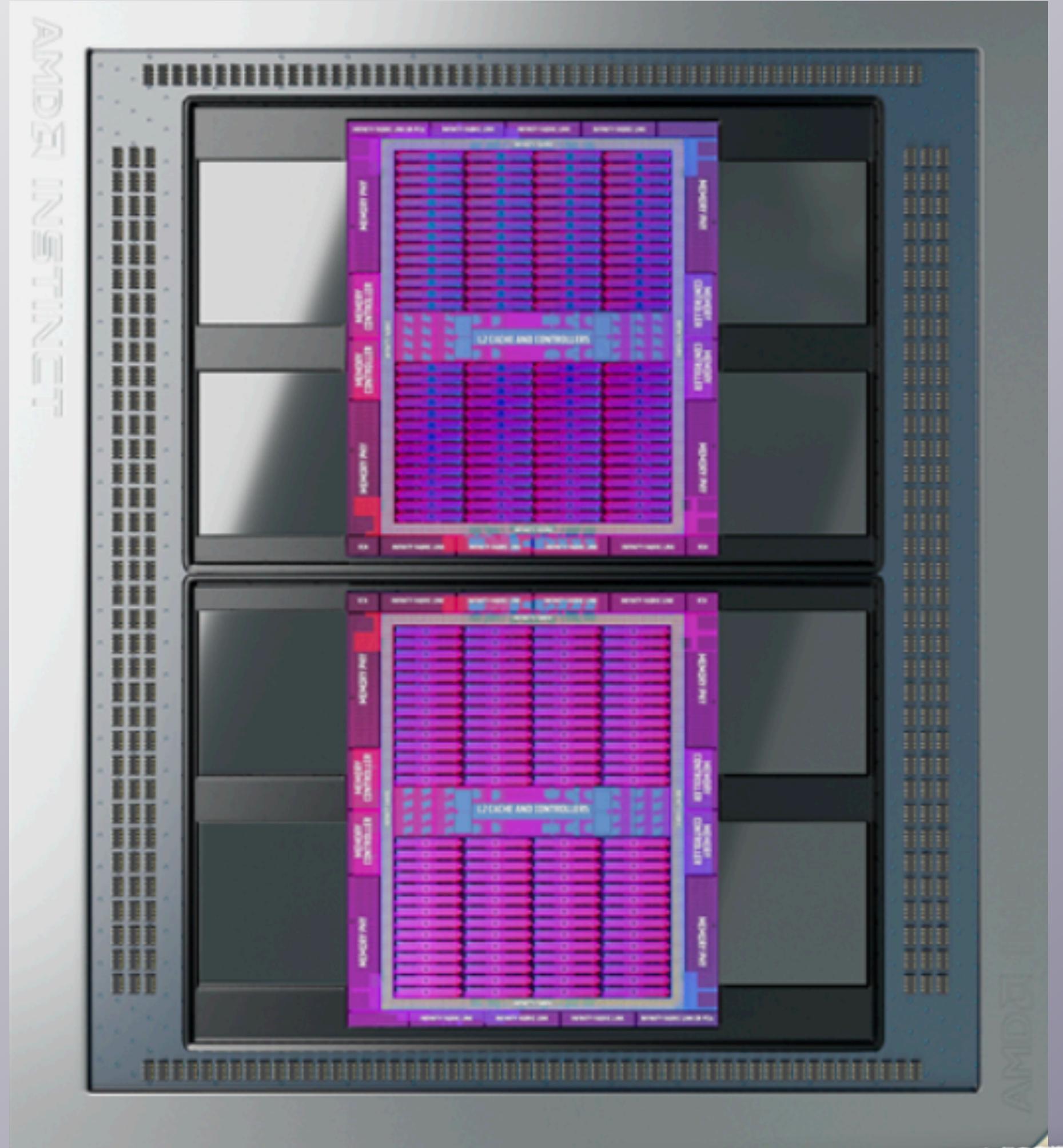
## Intel CPU/GPUs, AMD CPU/GPUs



These architectures will excel at AI + HPC



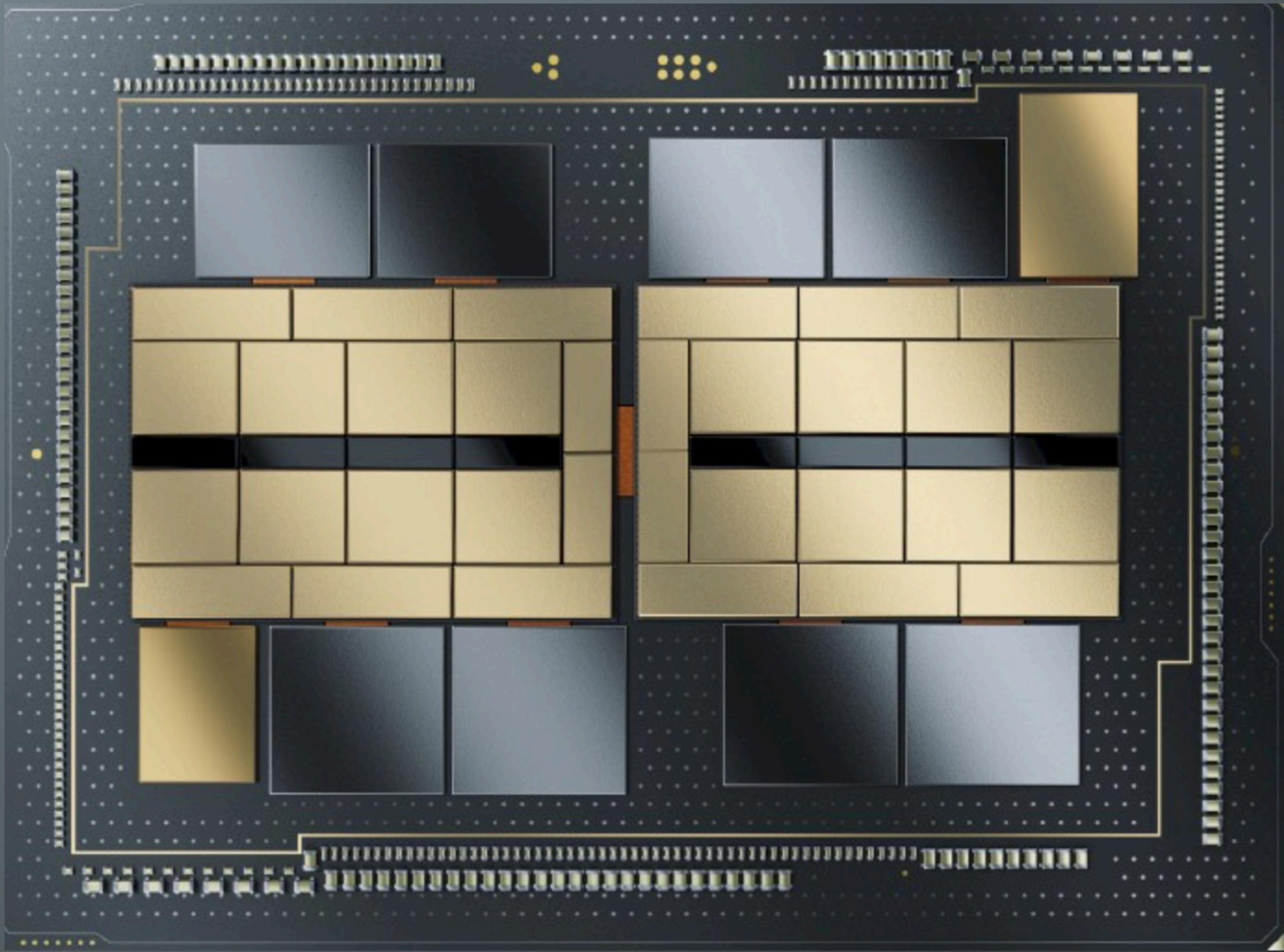
>2.3B Transistors  
58B transistors on TN6



Frontier  $\approx 4 \times 10^4$   
MI-250X (AMD)



>6B Transistors  
>100B transistors on TN5, (IN7, IN10)



Aurora  $\approx 6 \times 10^4$   
Xe (PVC) (Intel)





# Aurora<sup>1</sup>

Leadership Computing Facility  
Exascale Supercomputer

## PEAK PERFORMANCE

$\geq 2$  Exaflops DP

## Intel GPU

Ponte Vecchio

## Intel Xeon PROCESSOR

Sapphire Rapids + HBM

## PLATFORM

HPE Cray-Ex

### Compute Node

2 SPR+HBM processor;  
6 PVC; Unified  
Memory Architecture;  
8 fabric endpoints;

### GPU Architecture

Xe arch-based “Ponte  
Vecchio” GPU  
Tile-based chiplets  
HBM stack  
Foveros 3D integration

### System Interconnect

HPE Slingshot 11; Dragonfly  
topology with adaptive routing

### Network Switch

25.6 Tb/s per switch, from 64–200  
Gb/s ports (25 GB/s per direction)

### Node Performance

>130 TF

### System Size

>9,000 nodes

### Aggregate System Memory

>10 PB aggregate System  
Memory

### High-Performance Storage

**220 PB @ EC16+2,  $\geq 25$  TB/s**

### DAOS

### Programming Models

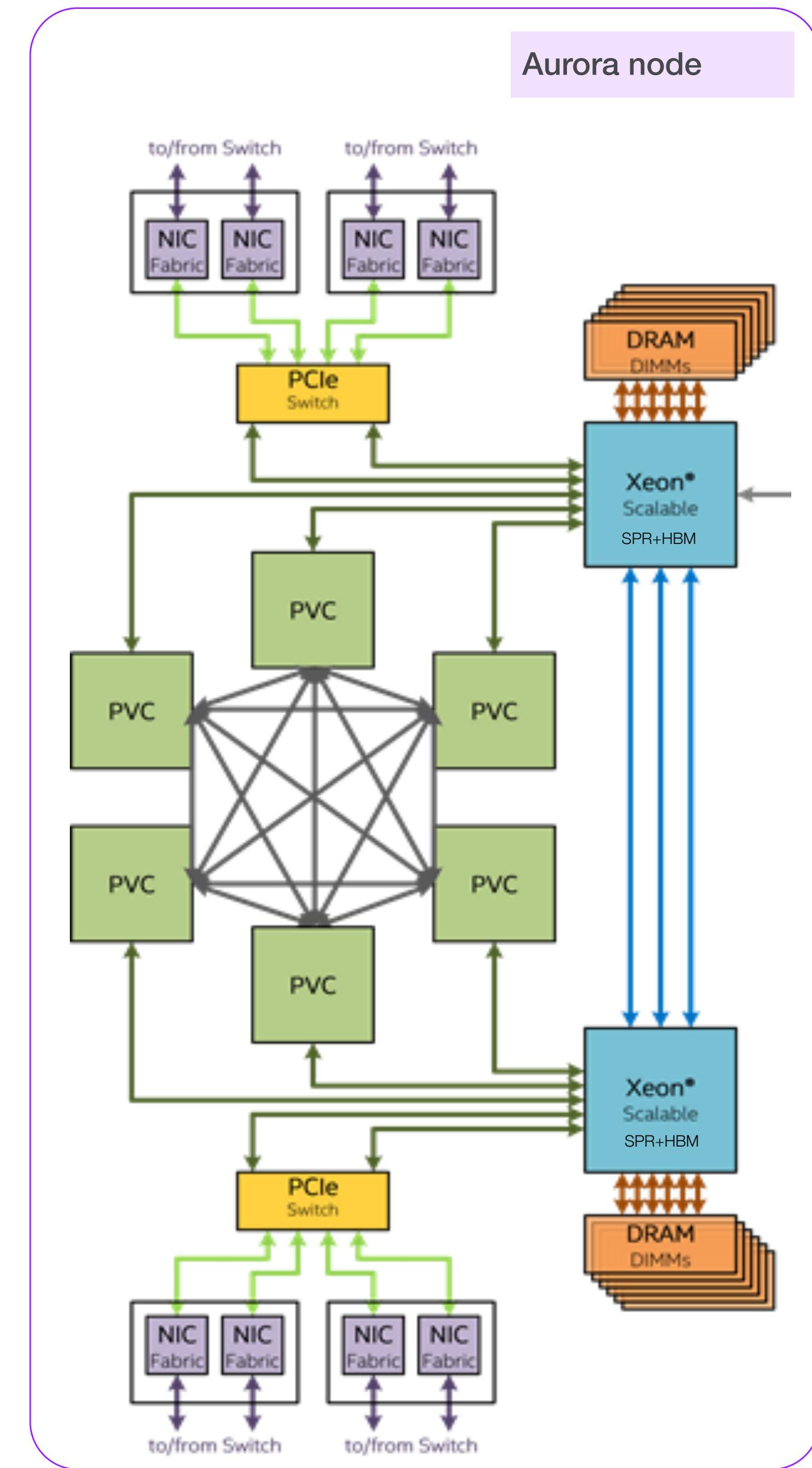
oneAPI, MPI, OpenMP, C/C++,  
Fortran, SYCL/DPC++  
Python-based environments

### ML + Deep learning frameworks

**1:** *The Computer That WILL Change Everything*

# Aurora Compute Node

- 6 X<sup>e</sup> Architecture based GPUs (Ponte Vecchio)
  - All to all connection
- 2 Intel Xeon (Sapphire Rapids) processors
- Unified Memory Architecture across CPUs and GPUs
- 8 Slingshot Fabric endpoints



# Aurora Cabinets Installed at Argonne



The Aurora Supercomputer at ALCF

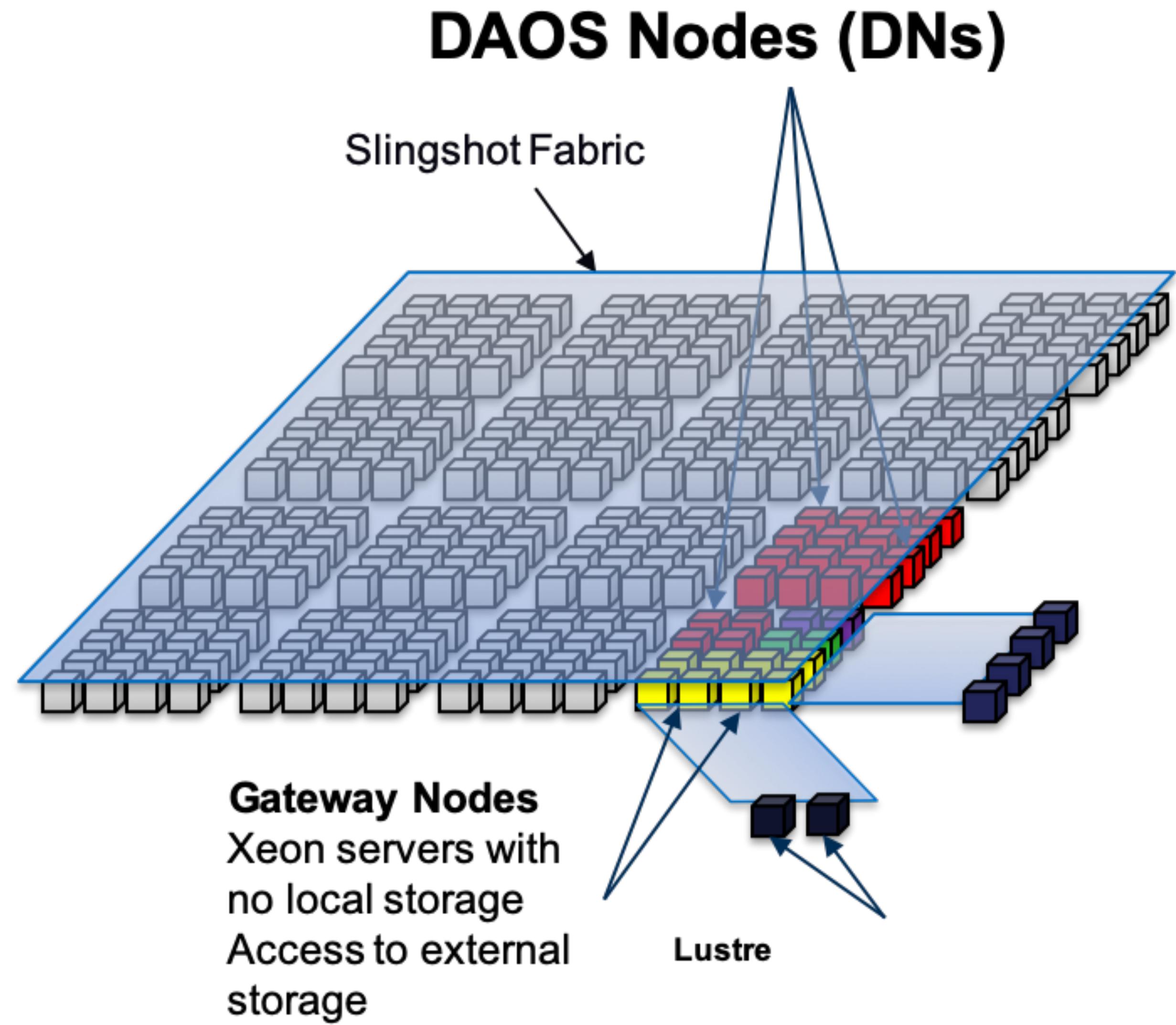


# Aurora

> 60,000 Intel GPUs  
Science Starts in 2023

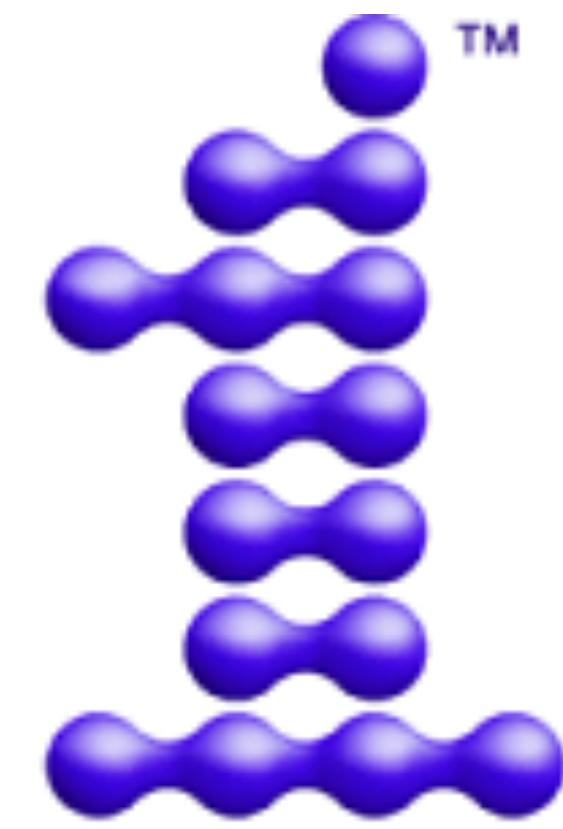
# Distributed Asynchronous Object Store (DAOS)

- Primary storage system for Aurora
- Offers high performance in bandwidth and IO operations
  - **230 PB capacity**
  - $\geq 25 \text{ TB/s}$
- Provides a flexible storage API that enables new I/O paradigms
- Provides compatibility with existing I/O models such as POSIX, MPI-IO and HDF5
- Open source storage solution



# oneAPI

- [Industry specification](#) from Intel
  - Language and libraries to target programming across diverse architectures (DPC++, APIs, low level interface)
- [Intel oneAPI](#) products and toolkits
  - **Languages**
    - Fortran (w/ OpenMP 5+)
    - C/C++ (w/ OpenMP 5+)
    - DPC++
    - Python
  - **Libraries**
    - oneAPI MKL (oneMKL)
    - oneAPI Deep Neural Network Library (oneDNN)
    - oneAPI Data Analytics Library (oneDAL)
    - MPI
  - **Tools**
    - Intel Advisor
    - Intel VTune
    - Intel Inspector



# oneAPI

<https://software.intel.com/oneapi>

# Available Aurora Programming Models

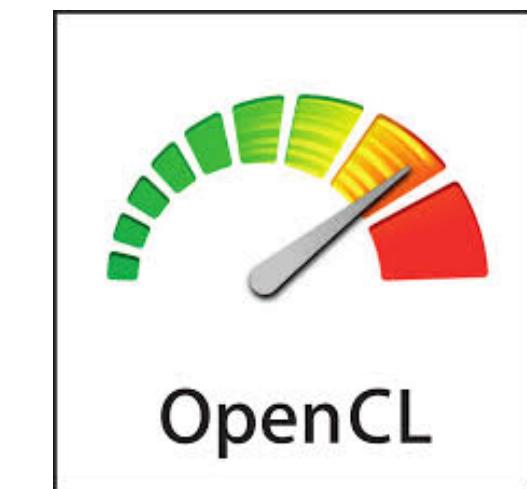
- Aurora applications may use:
  - DPC++/SYCL
  - OpenMP
  - Kokkos
  - Raja
  - OpenCL
- Experimental
  - HIP
- Not available on Aurora:
  - ~~CUDA~~
  - ~~OpenACC~~



**RAJA**

**HIP**

**OpenMP**

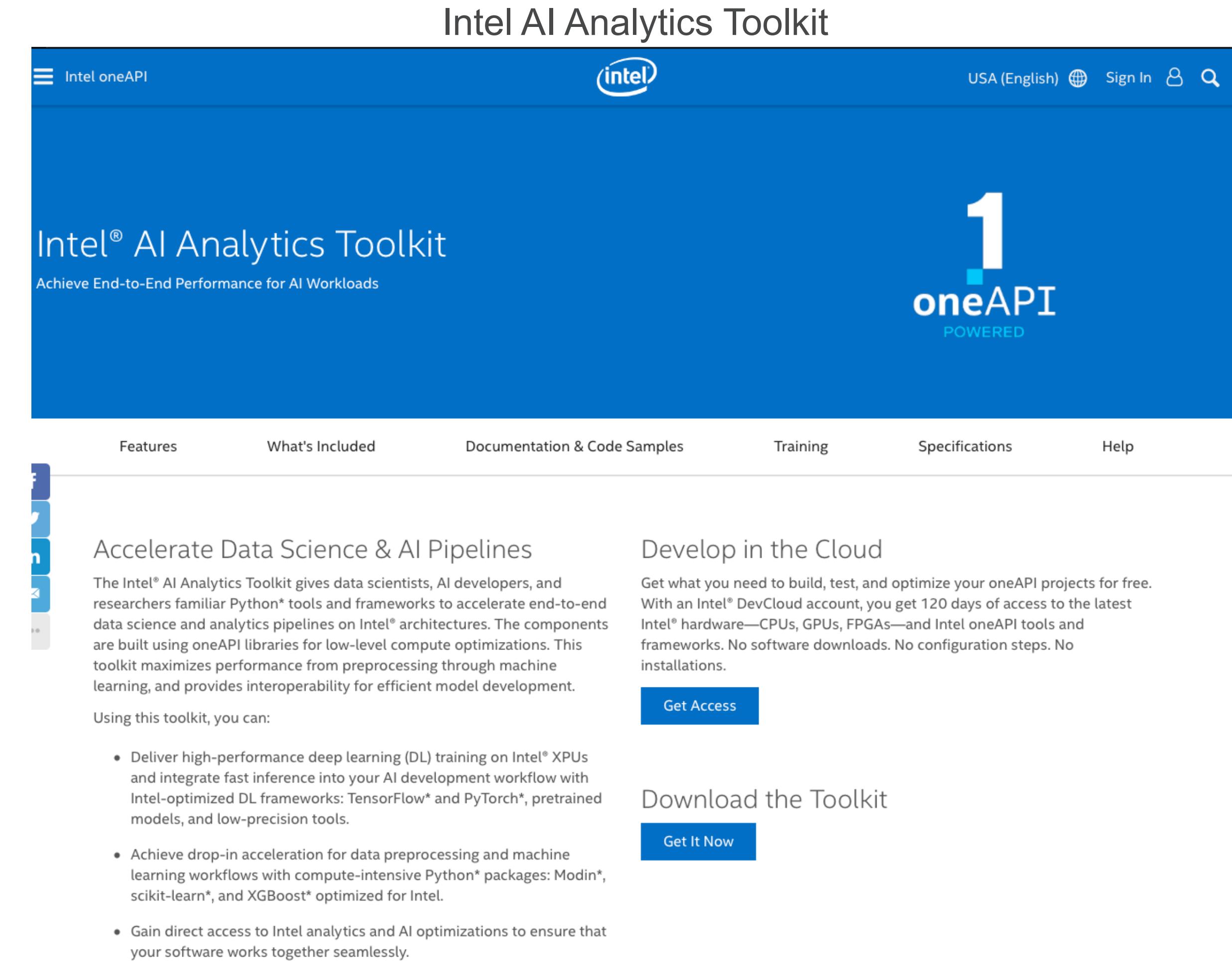


# Data Science and Learning on Aurora

Aurora Will Provide for a Familiar, Productive and Performant HPC and AI Software Stack

- Python Ecosystem:
  - Numba, NumPy, etc.
- **ML + Deep Learning Frameworks:**
  - OneDAL, scikit-learn, XGBoost, etc.
  - PyTorch, TensorFlow,  
Horovod, DDP, DeepSpeed, 
  - Accelerate
- *Optimized + scalable communication* with OneCCL
- Spark BigData Analytics
- DAOS for fast I/O + workflows
- Profiling and debugging tools

Intel AI Analytics Toolkit



Intel oneAPI      intel      USA (English)      Sign In      Q

1  
oneAPI  
POWERED

Features      What's Included      Documentation & Code Samples      Training      Specifications      Help

Accelerate Data Science & AI Pipelines

The Intel® AI Analytics Toolkit gives data scientists, AI developers, and researchers familiar Python\* tools and frameworks to accelerate end-to-end data science and analytics pipelines on Intel® architectures. The components are built using oneAPI libraries for low-level compute optimizations. This toolkit maximizes performance from preprocessing through machine learning, and provides interoperability for efficient model development.

Using this toolkit, you can:

- Deliver high-performance deep learning (DL) training on Intel® XPU and integrate fast inference into your AI development workflow with Intel-optimized DL frameworks: TensorFlow\* and PyTorch\*, pretrained models, and low-precision tools.
- Achieve drop-in acceleration for data preprocessing and machine learning workflows with compute-intensive Python\* packages: Modin\*, scikit-learn\*, and XGBoost\* optimized for Intel.
- Gain direct access to Intel analytics and AI optimizations to ensure that your software works together seamlessly.

Develop in the Cloud

Get what you need to build, test, and optimize your oneAPI projects for free. With an Intel® DevCloud account, you get 120 days of access to the latest Intel® hardware—CPUs, GPUs, FPGAs—and Intel oneAPI tools and frameworks. No software downloads. No configuration steps. No installations.

Get Access

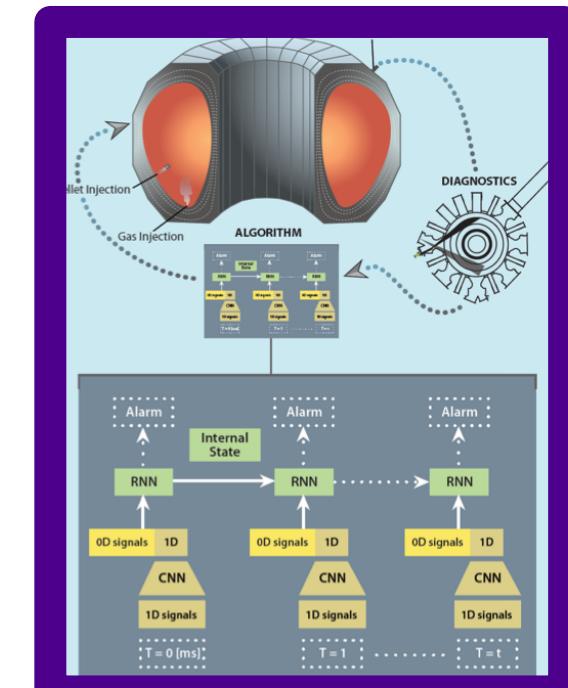
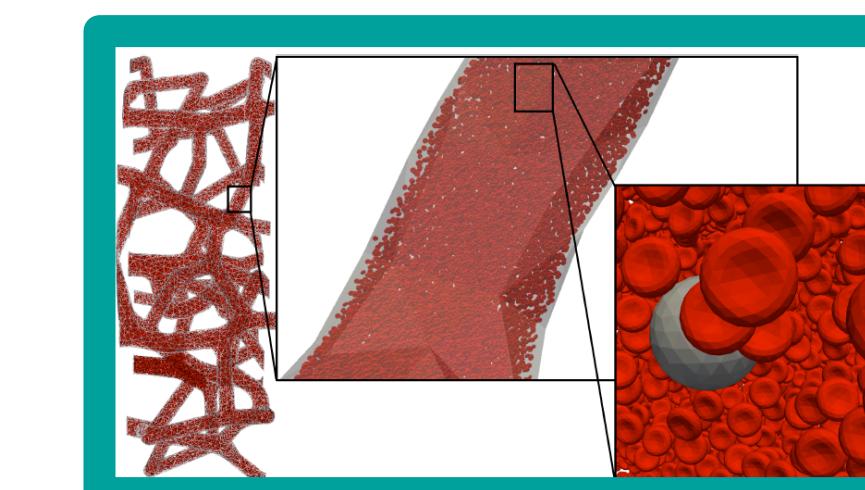
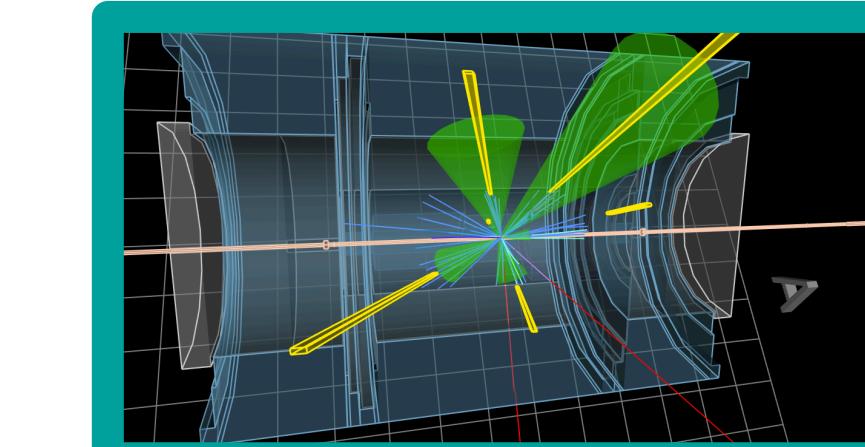
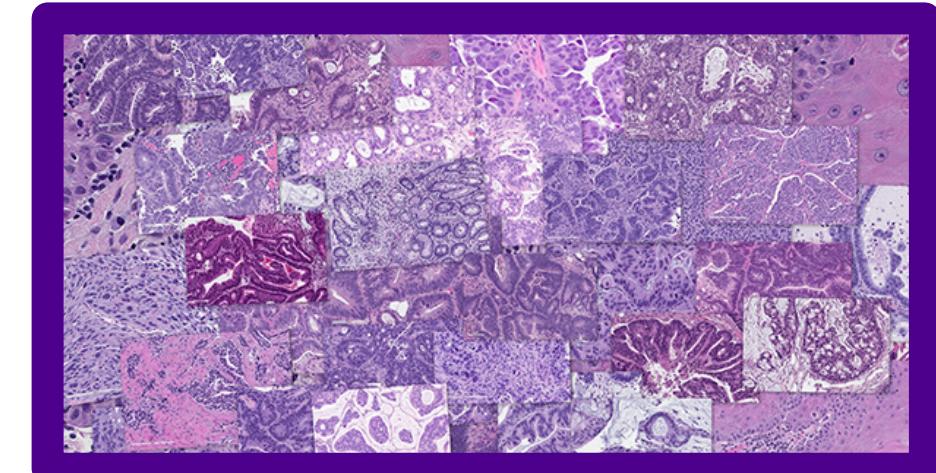
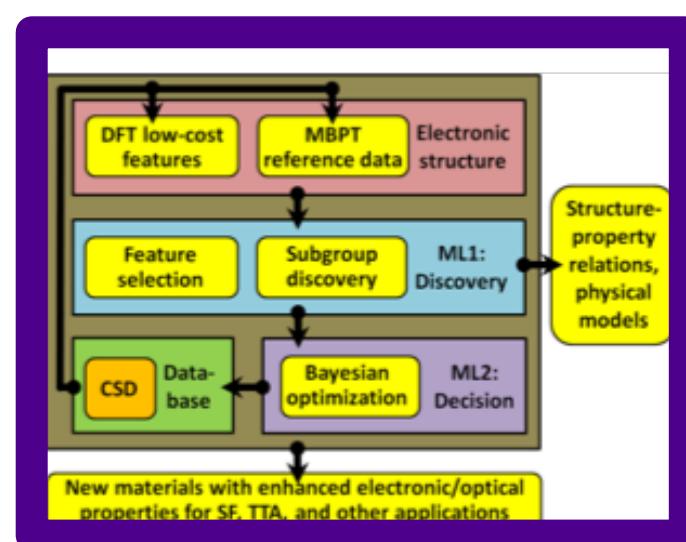
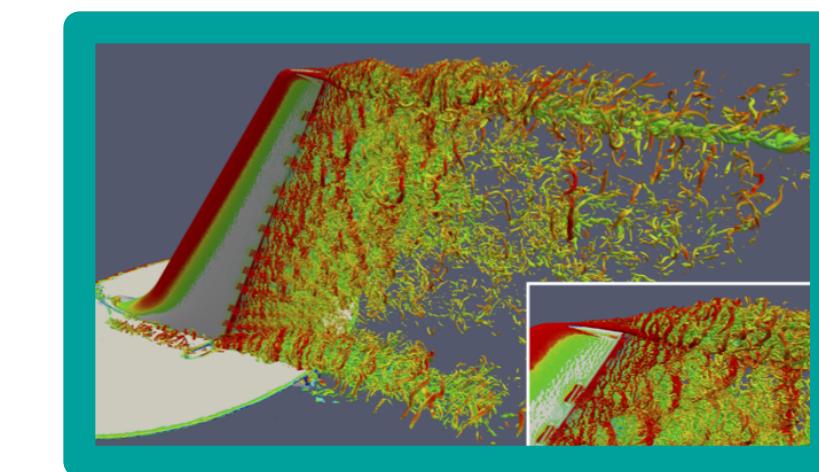
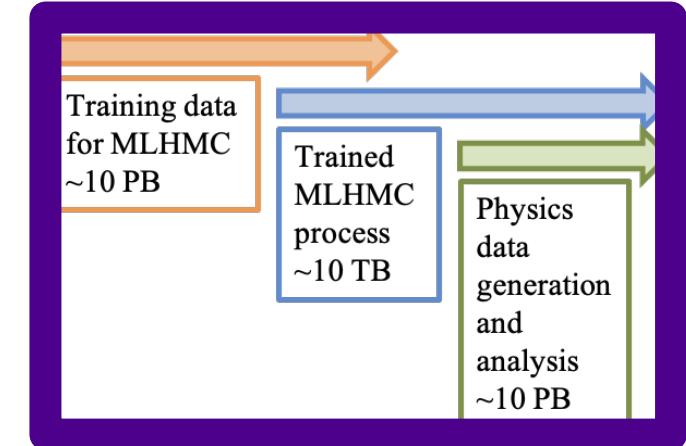
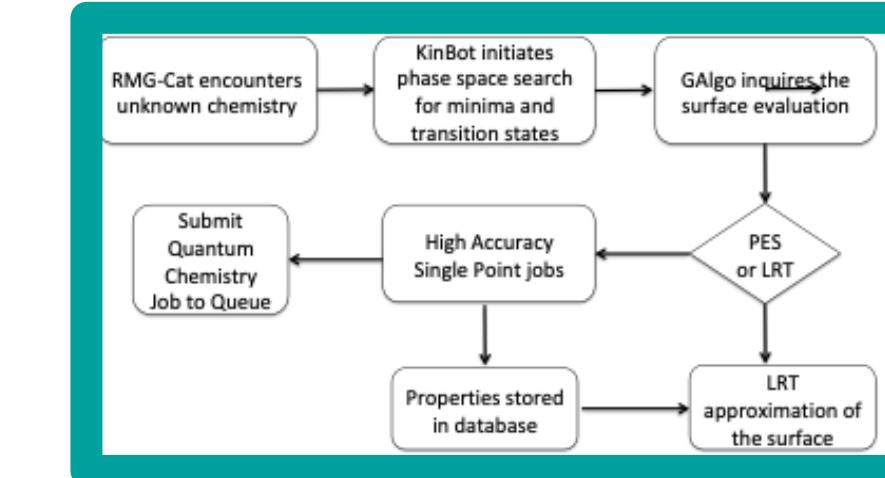
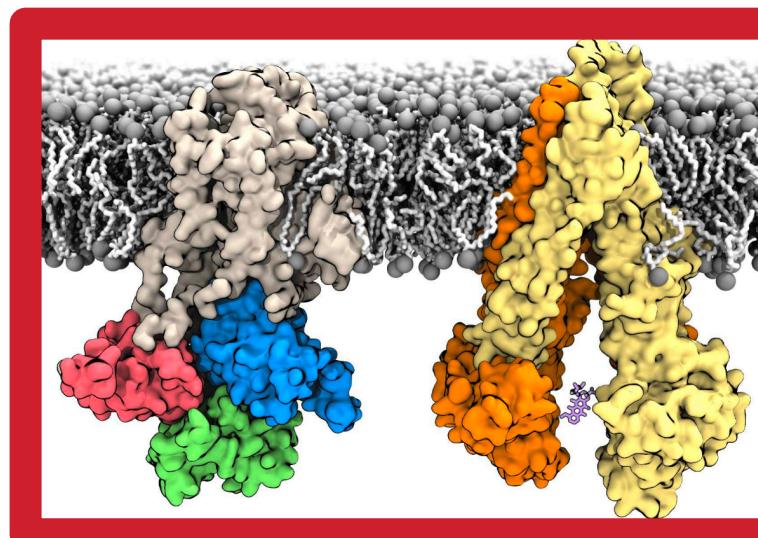
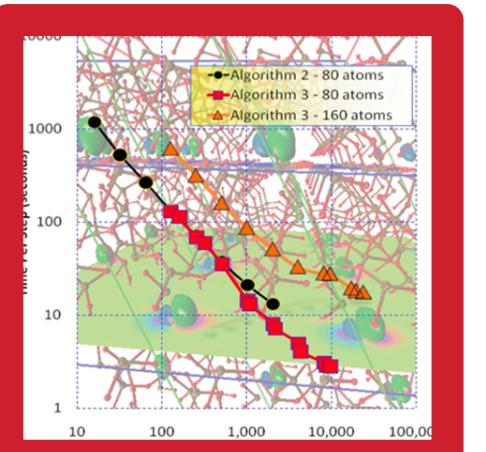
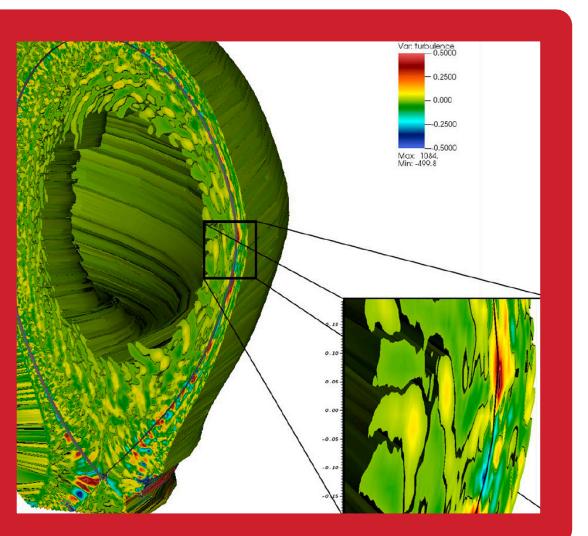
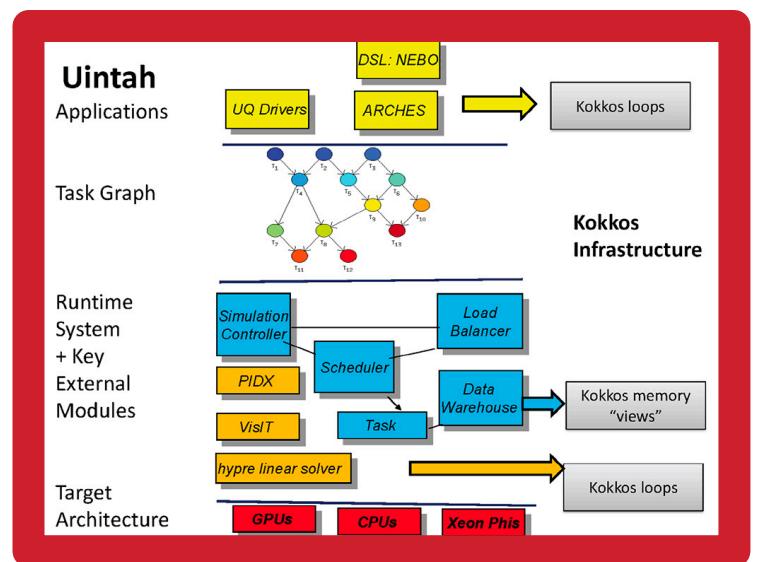
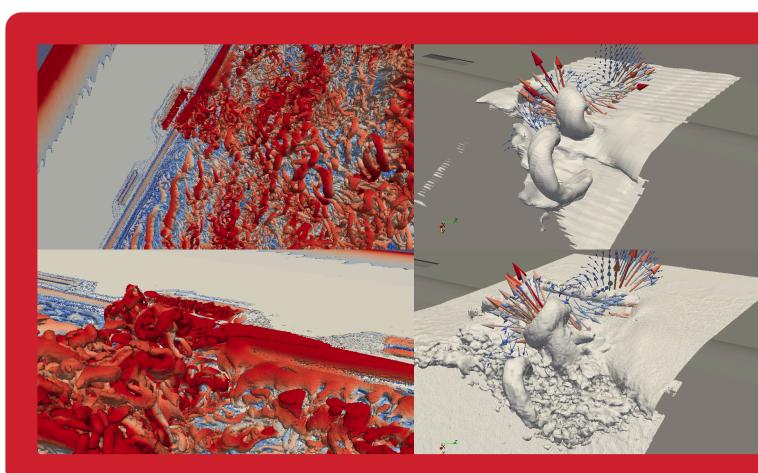
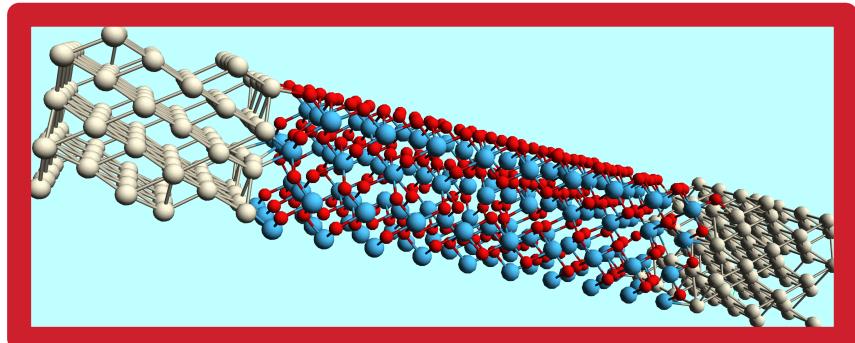
Download the Toolkit

Get It Now

<https://software.intel.com/content/www/us/en/develop/tools/oneapi/ai-analytics-toolkit.html>

# Aurora ESP Projects

S D L



# Aurora ESP Projects

S D L

**Anouar Benali** (ANL)

Extending Moore's Law computing with Quantum Monte Carlo

**Martin Berzins** (U. Utah)

Design & evaluation of high-efficiency boilers for energy production using a hierarchical V/UQ approach

**CS Chang** (PPPL)

High fidelity simulation of fusion reactor boundary plasmas

**Theresa Windus** (Ames)

NWChemEx: Tackling Chemical, Materials & Biochemical Challenges in the Exascale Era

**Katrin Heitmann** (ANL)

Extreme-Scale Cosmological Hydrodynamics

**Ken Jansen** (U. Colorado)

Extreme Scale Unstructured Adaptive CFD: From Multiphase Flow to Aerodynamic Flow Control

**Norman Christ** (Columbia)

Lattice Quantum Chromodynamics Calculations for Particle and Nuclear Physics

**Aiichiro Nakano** (USC)

Metascalable Layered Materials Genome

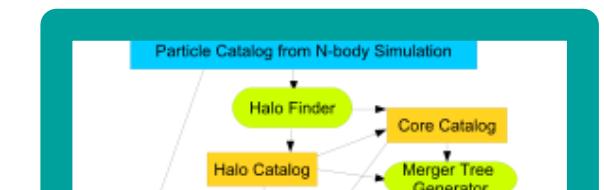
**Benoit Roux** (U. Chicago)

Free Energy Landscapes of Membrane Transport Proteins

**David Bross** (ANL)

Exascale Computational Catalysis

IN database the surface



**Salman Habib** (ANL)

Dark Sky Mining

**Ken Jansen** (U. Colorado)

Data Analytics and Machine Learning for Exascale CFD

**Walter Hopkins** (ANL)

Simulating and Learning in the ATLAS detector at the Exascale

**Amanda Randles** (Duke U.)

Extreme-scale In Situ Visualization and Analysis of Fluid-Structure-Interaction Simulations

**Will Detmold** (MIT)

Machine Learning for Lattice Quantum Chromodynamics

**Nicola Ferrier** (ANL)

Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience

**Noa Marom** (CMU)

Many-Body Perturbation Theory Meets Machine Learning to Discover Singlet Fission Materials

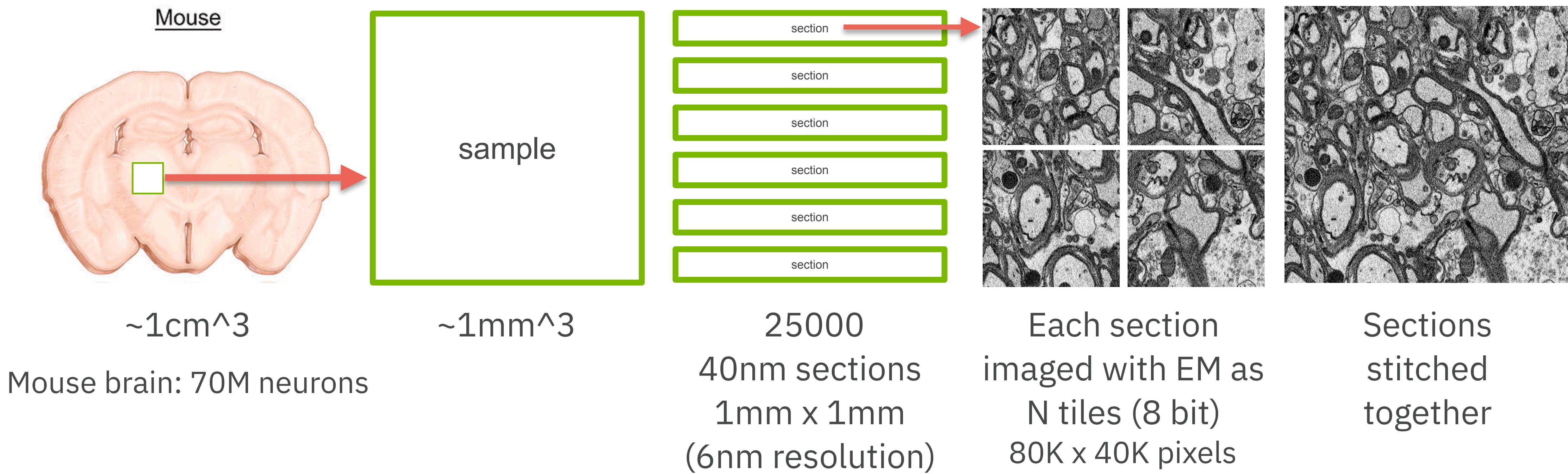
**Rick Stevens** (ANL)

Virtual Drug Response Prediction

**Bill Tang** (Princeton)

Accelerated Deep Learning Discovery in Fusion Energy Science

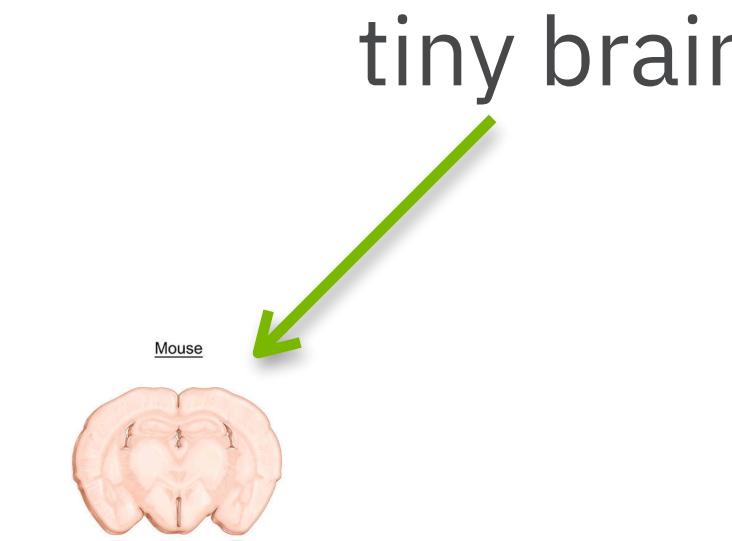
# Connectomics Data-Driven Models



How much image data is  $1\text{mm}^3$ ?  $1 \times 10^{15}$  voxels --> ~1 PB

# Data Challenges in Connectomics

**Mouse brain: 70M neurons**



$\sim 1\text{cm}^3$

How much image data  
is  $1\text{cm}^3$  ?  **$\sim 1\text{EB}$**

**Human brain: 80B neurons**



$\sim 1000\text{cm}^3$

How much image data is  
 $1000\text{cm}^3$  ?  **$\sim 1000 \text{ EB}$**   
( $6\text{nm} \times 6\text{nm} \times 40\text{nm}$ )

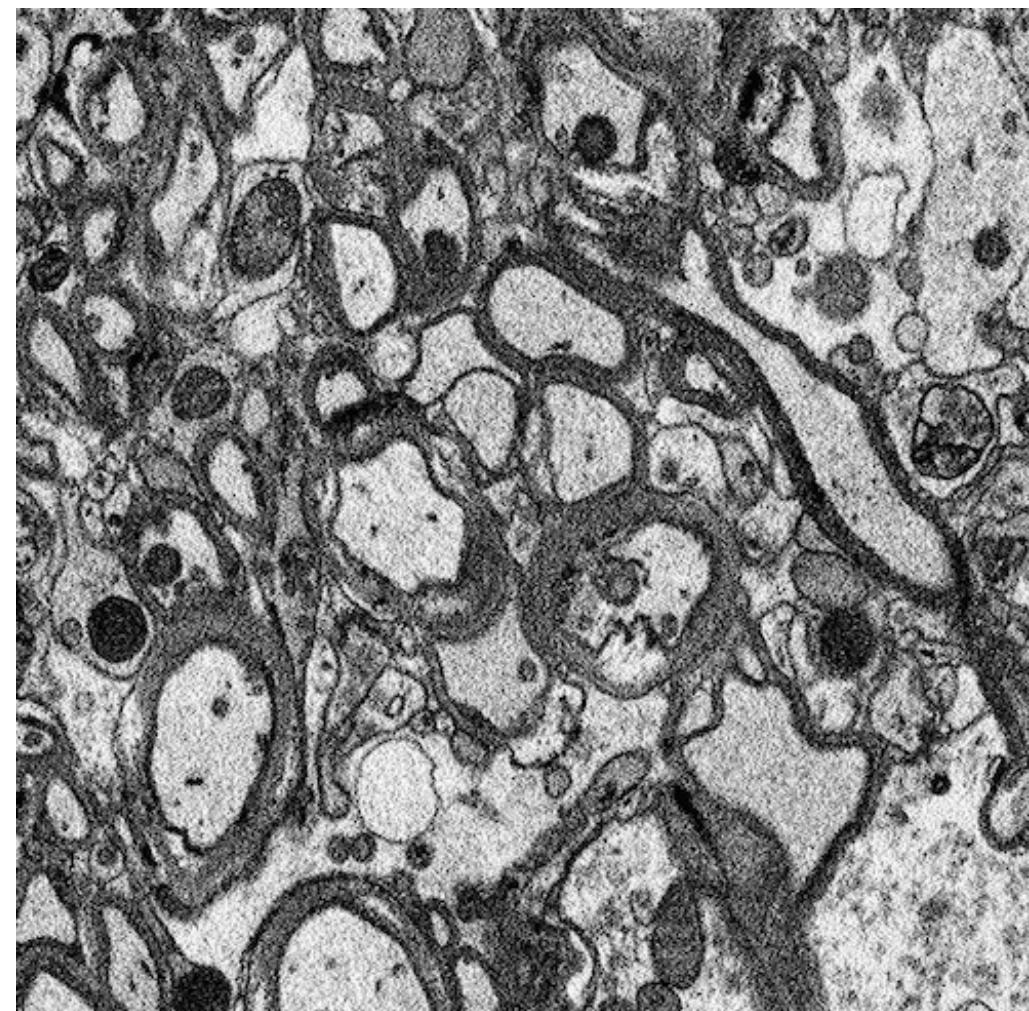
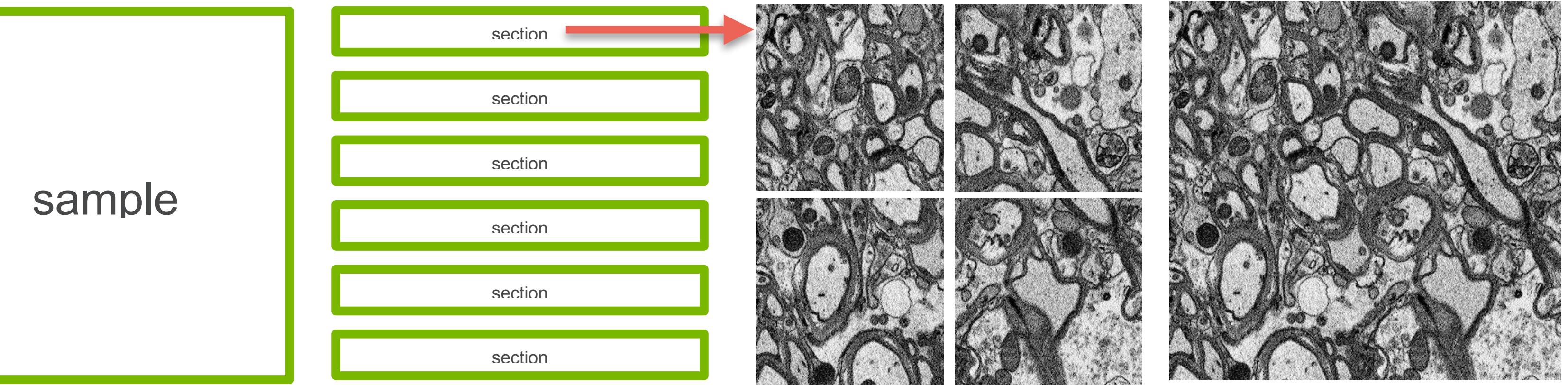
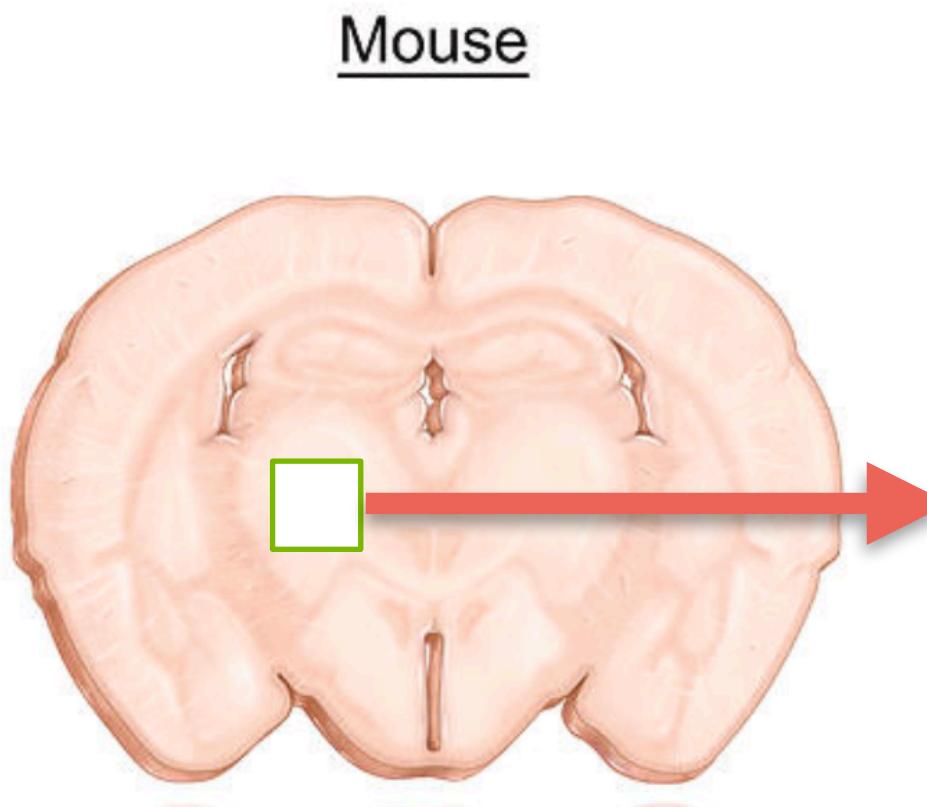


**Reconstructed data  
will be much larger:**

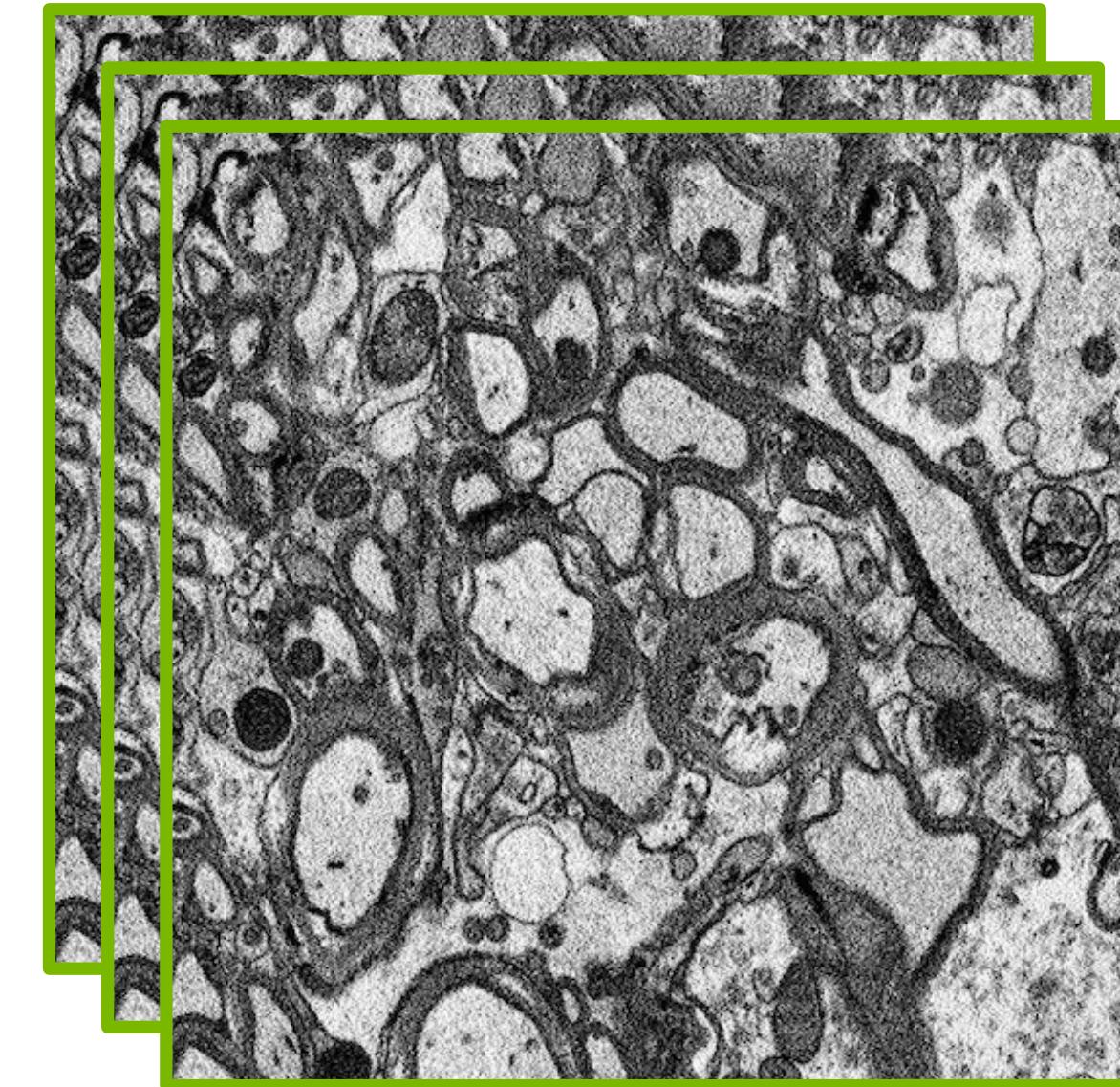
- Segmentation labels  
for each voxel
  - 4x voxel data
  - 3D Mesh
  - Skeleton

The structures are expected to  
be used to seed simulations to  
study flow in neurotransmitters,  
in better modeling the brain,  
among others.

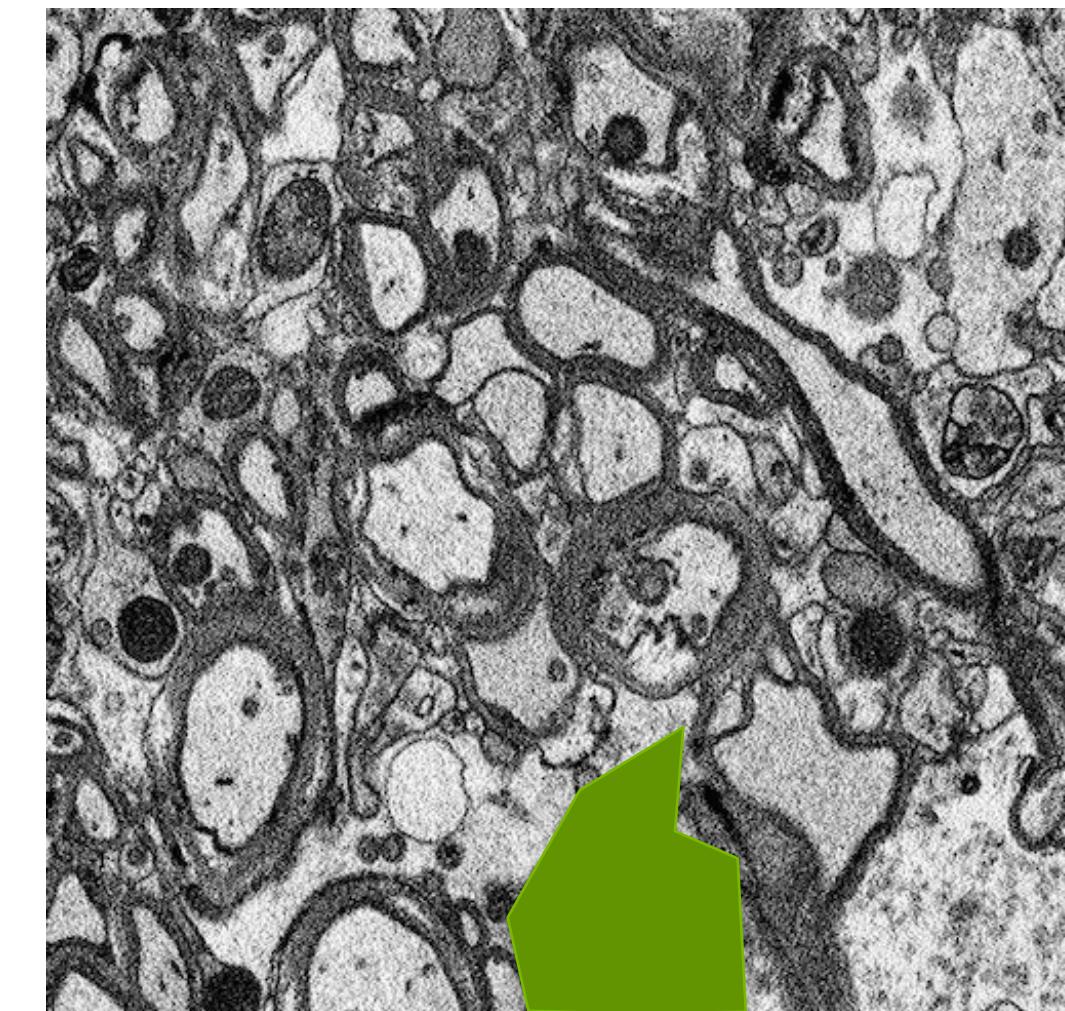
# Connectomics Processing



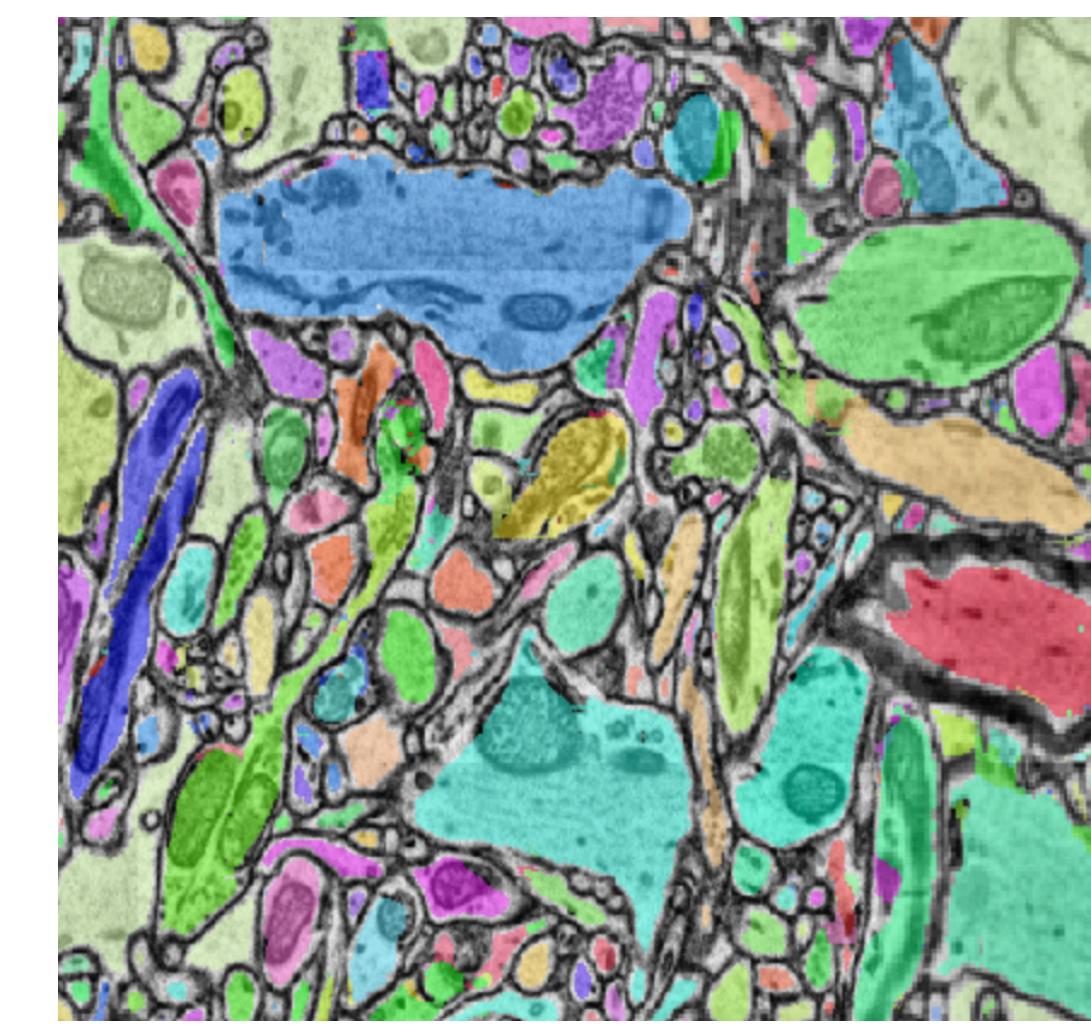
Sections stitched together



Align sections



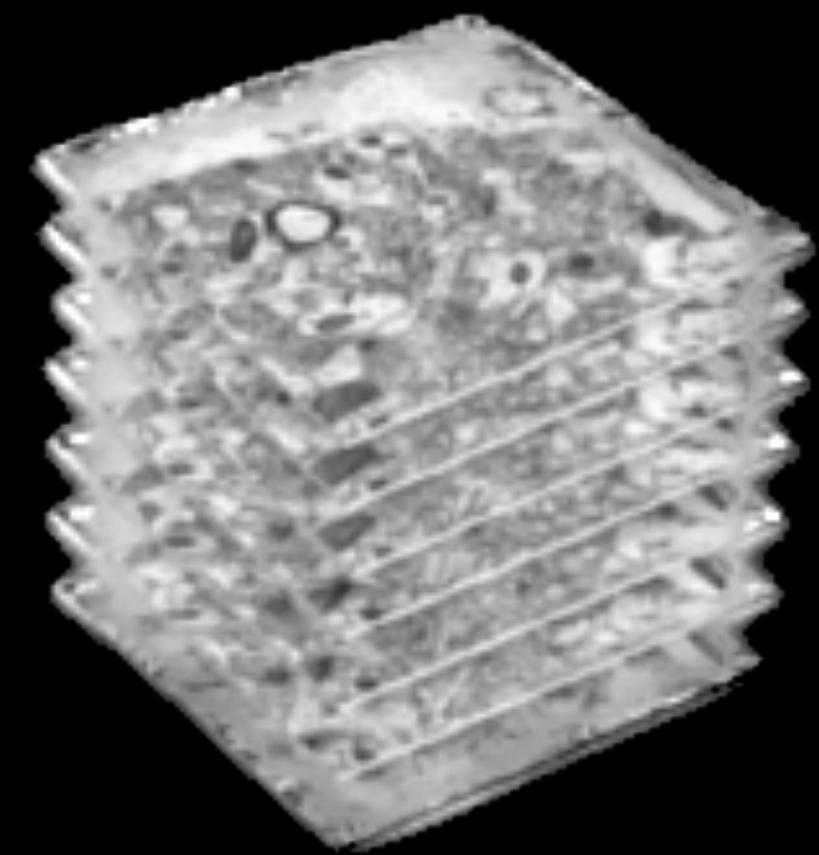
Mask out non-target objects



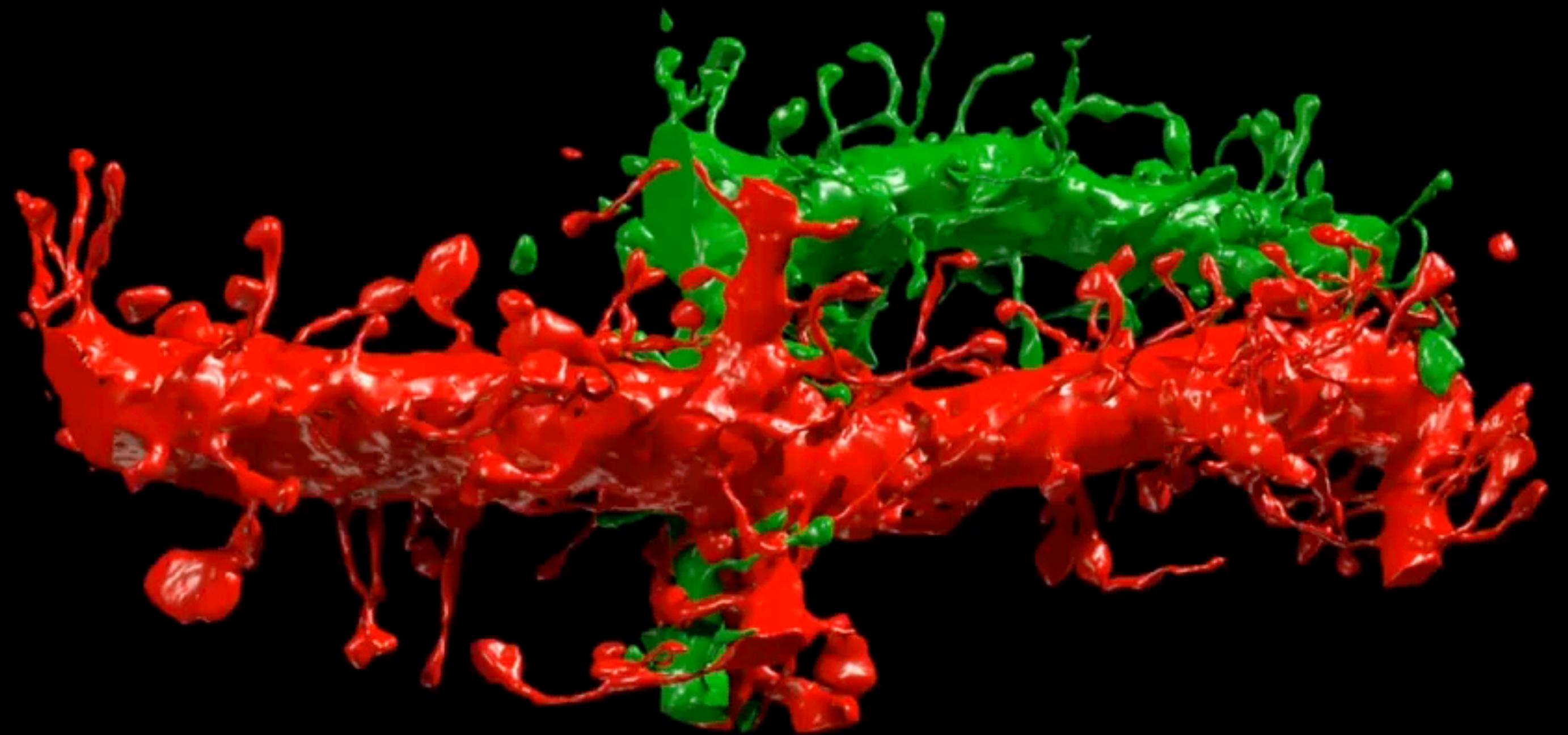
Segment target objects

# Reconstructing the Brain Connectivity

Kasthuri et al, Cell 2015



EM Images

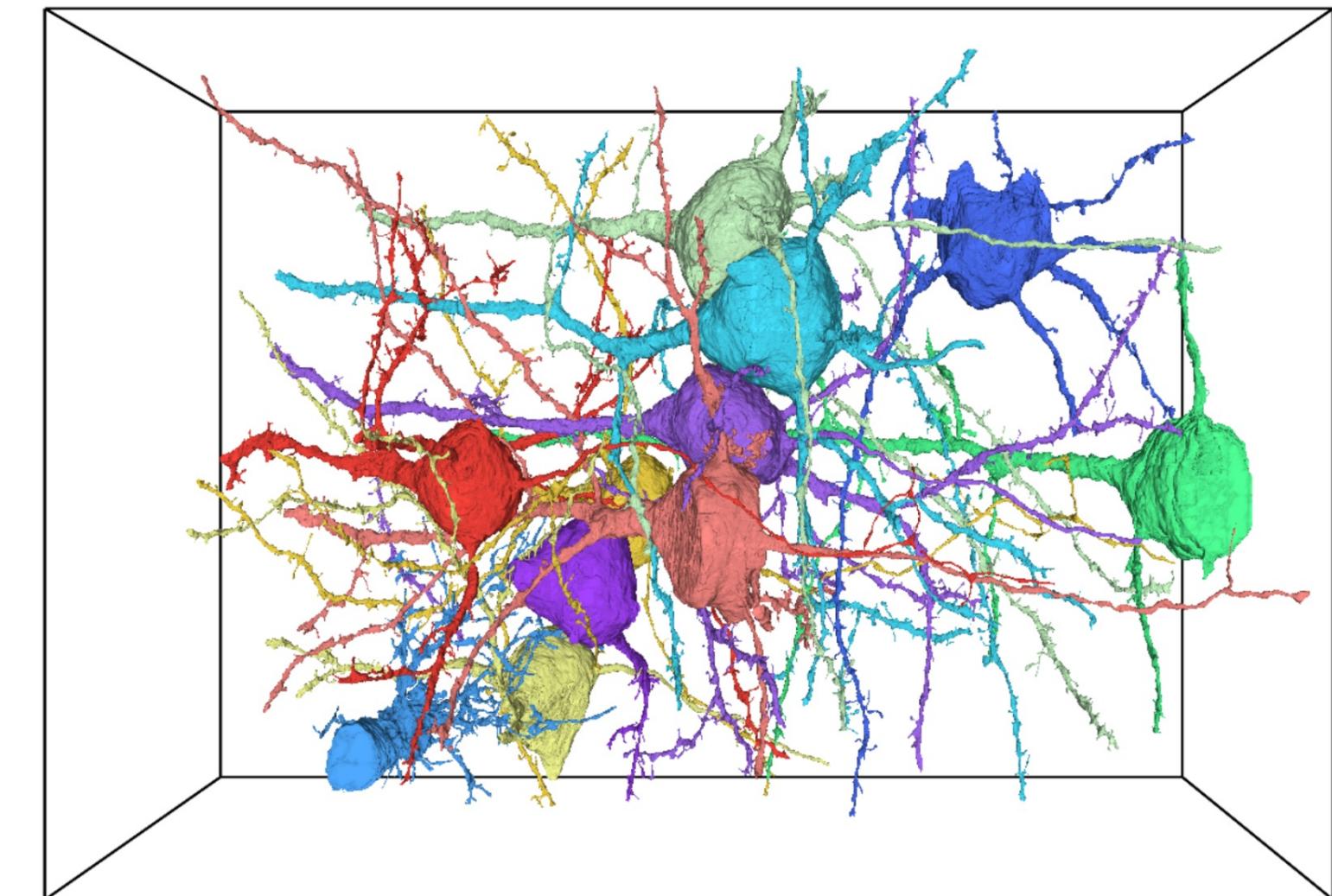
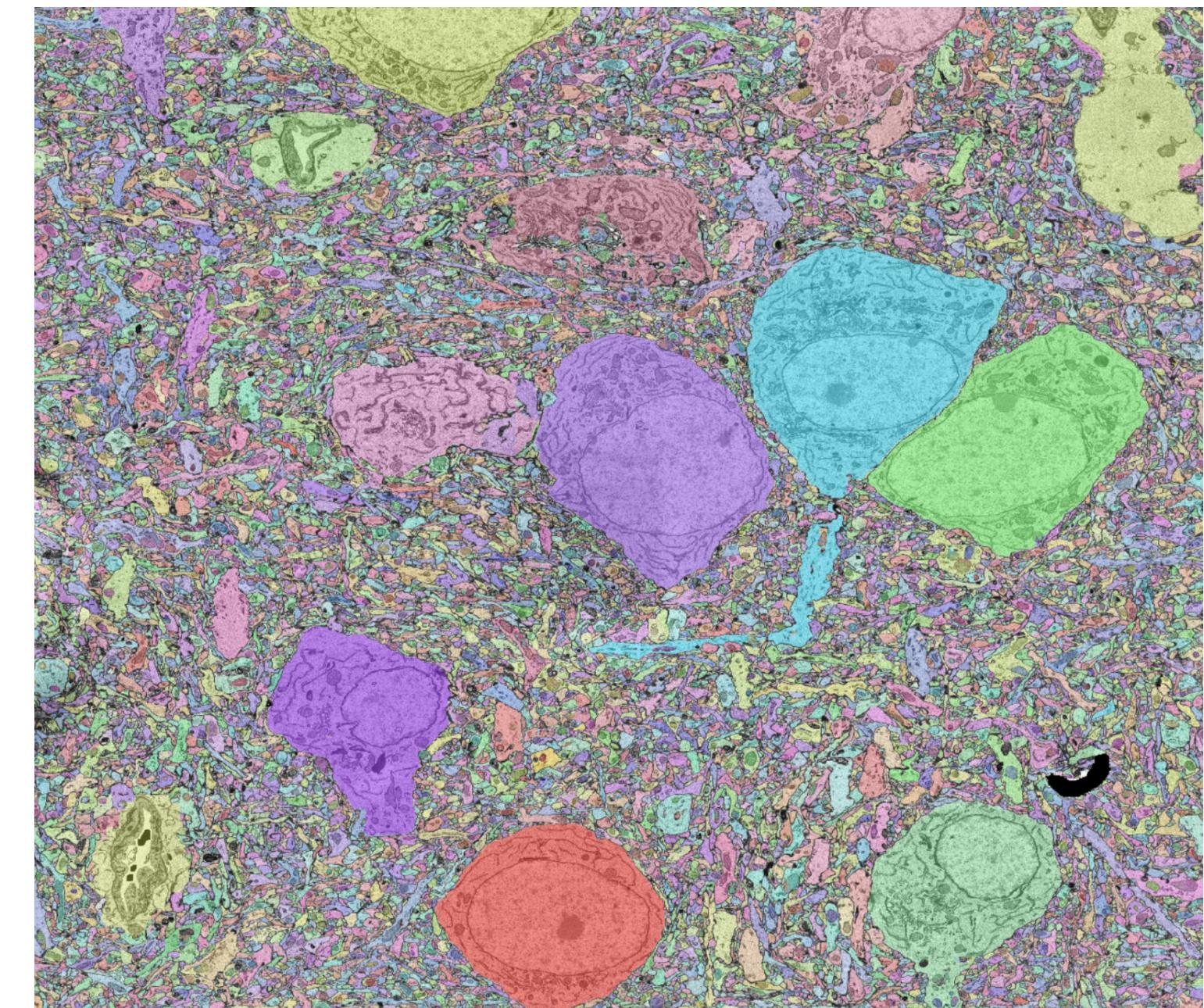


# Large-Scale Reconstruction

- Inference (and training) has scaled on CPU-based and GPU-based supercomputers (parallel granularity: overlapping subvolumes)
  - Achieved million-way concurrency on Theta supercomputer
- Image stitching and alignment components are being scaled as well to ensure a scalable end-to-end pipeline

## Exascale Inference Problem:

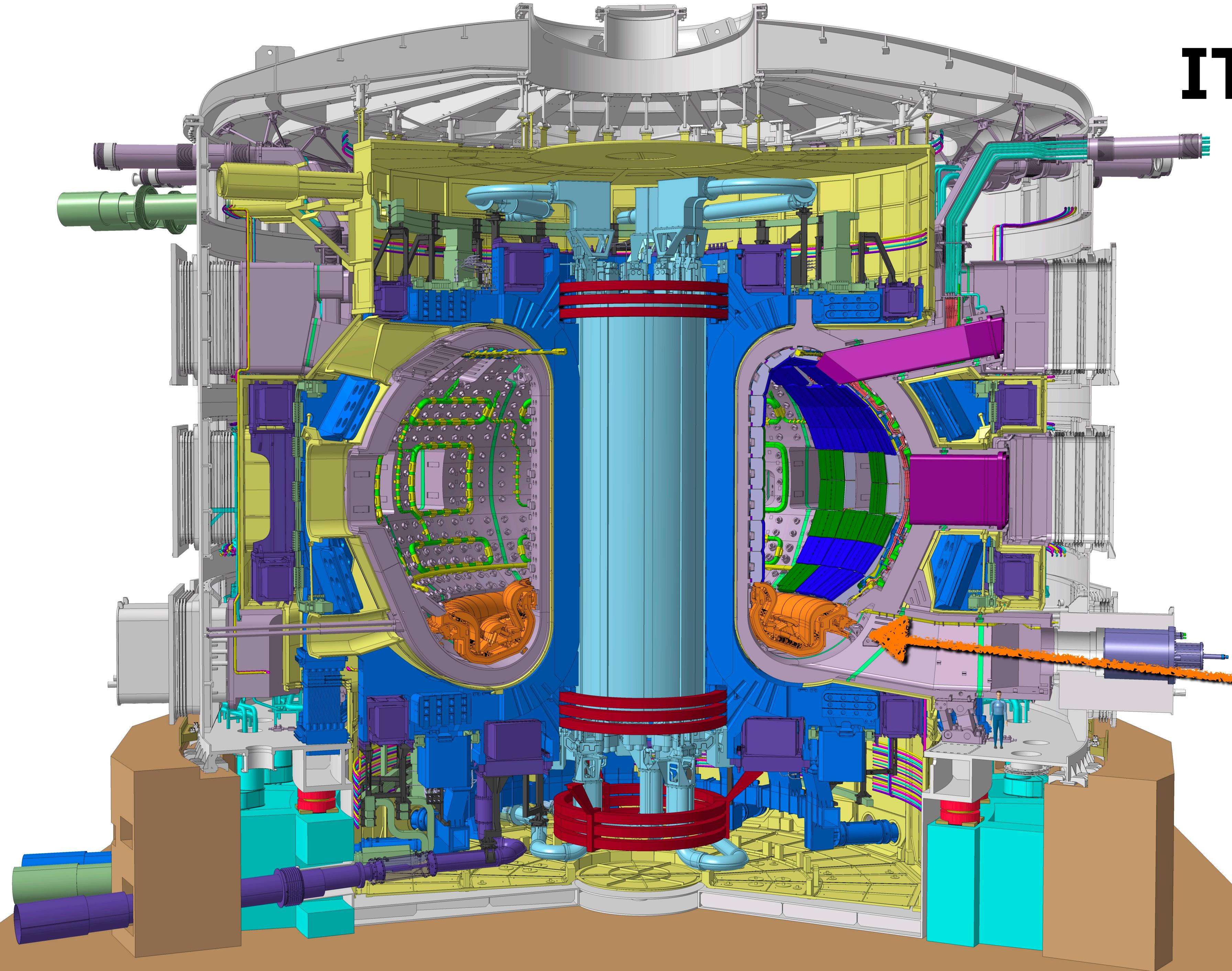
- On a single GPU (A100), we achieve ~80 MegaVoxels/hour using 32-bit (There is still room for improvement here)
- In reduced precision (8-16 bits), we expect ~1 GigaVoxel/hour per GPU
- 1 PetaVoxel ( $1\text{mm}^3$ ) will take ~1M GPU node hours
- Approximately, **24 hours on a system with 50K GPUs** (considering overlapping sub-volumes)
- For a mouse brain ( $1\text{cm}^3$ ), 1 ExaVoxel, we would need **~3 years on an exascale system**



Dong, et al, “Scaling Distributed Training of Flood-Filling Networks on HPC Infrastructure for Brain Mapping”, 2019 IEEE/ACM Third Workshop on Deep Learning on Supercomputers (DLS) at SC19

Vescovi, et al, “Toward an Automated HPC Pipeline for Processing Large Scale Electron Microscopy Data”, 2020 IEEE/ACM 2nd Annual Workshop on Extreme-scale Experiment-in-the-Loop Computing (XLOOP) at SC19

# ITER Tokamak



Predict ITER plasma  
behavior with  
Tungsten impurity  
ions

Divertor  
Tungsten

# Showcase

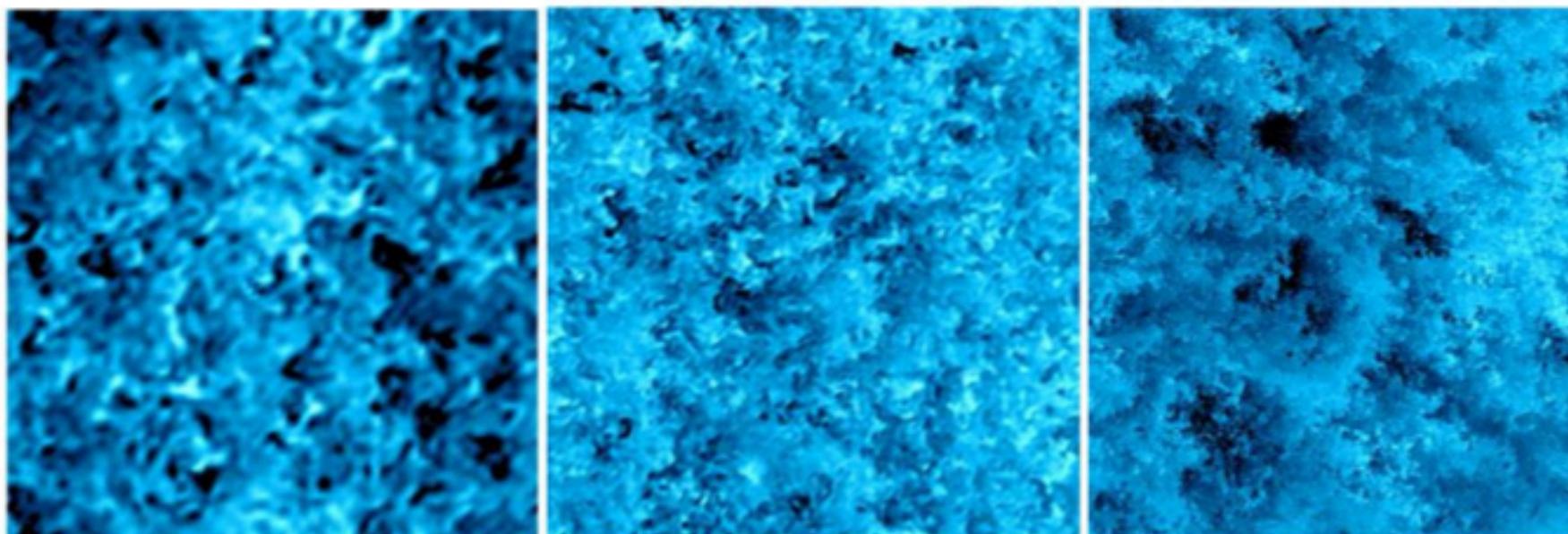
## ExaSMR: NekRS Performance on Ponte Vecchio

### Ponte Vecchio with Intel OneAPI DPC++ implementation

1.5x performance lead

**ExaSMR:** Small modular reactors (SMRs) and advanced reactor concepts (ARCs) will deliver clean, flexible, reliable, and affordable electricity while avoiding the traditional limitations of large nuclear reactor designs,

<https://www.exascaleproject.org/research-project/exasmr/>



**Figure 10:** NekRS: potential temperature distributions in [K] at time 6h and  $z=100\text{m}$  on different resolutions of  $\Delta x = 3.12\text{m}$  (left),  $1.56\text{m}$  (center), and  $0.78\text{m}$  (right) corresponding to the number of grid points,  $n=128^3$ ,  $256^3$ , and  $512^3$ , respectively.  $\Delta x$  represents the average grid-spacing for the spectral elements,  $E = 16^3$ ,  $32^3$  and  $64^3$  and the polynomial order  $N = 8$  on the domain  $400\text{m} \times 400\text{m} \times 400\text{m}$ .

<https://ceedexascaleproject.org/docs/ceed-ms38-report.pdf>

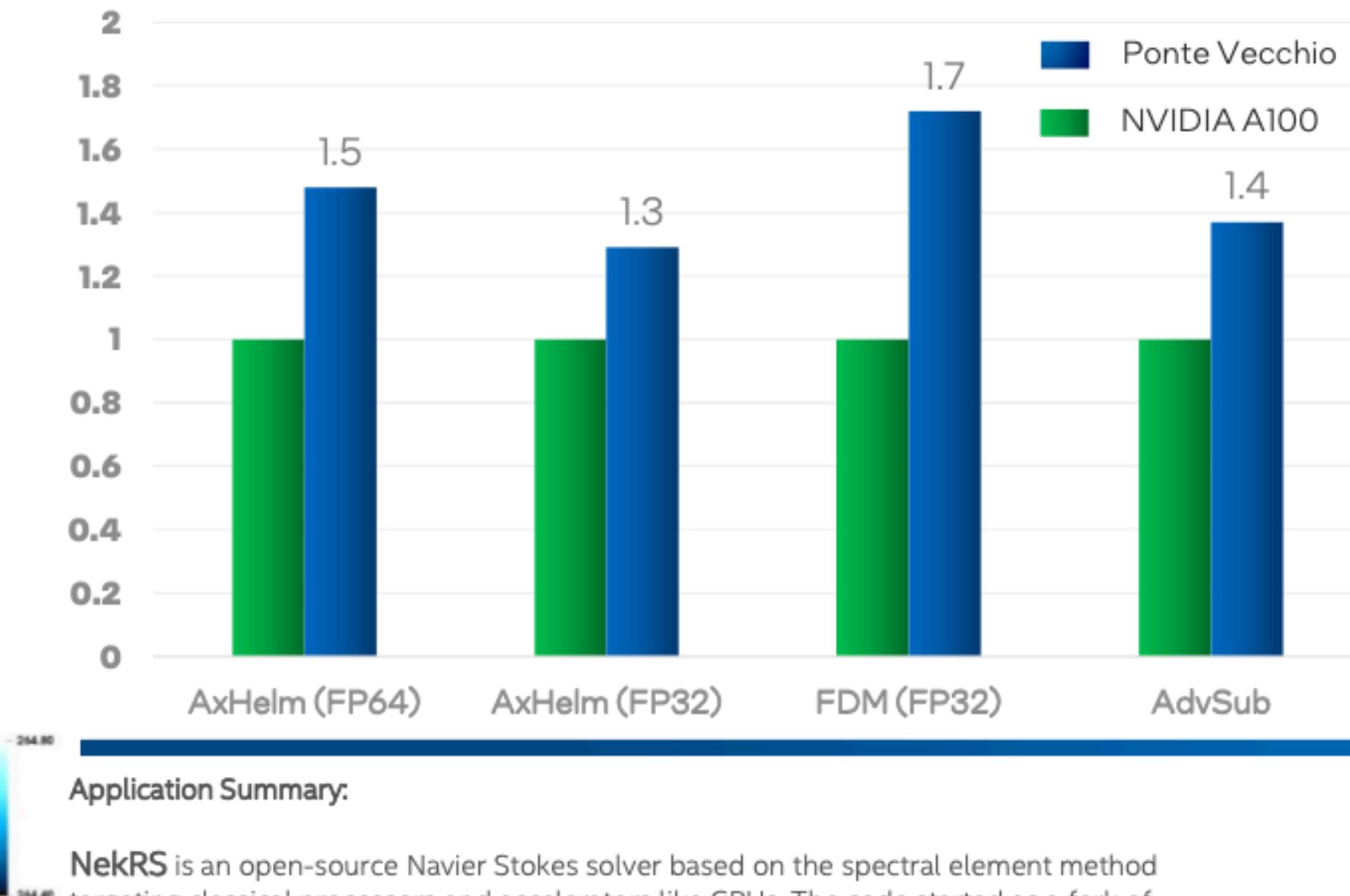


- See backup for workloads and configurations. Results may vary.
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Relative Performance of NekRS Benchmarks w/ problem size of 8196 (Averaged throughput, higher is better)



### Application Summary:

**NekRS** is an open-source Navier Stokes solver based on the spectral element method targeting classical processors and accelerators like GPUs. The code started as a fork of libParanumal in 2019. For API portable programming OCCA is used.

<https://github.com/argonne-lcf/nekRS/>

**OCCA** is an open-source library which aims to make it easy to program different types of devices (e.g. CPU, GPU, FPGA). It provides a unified API for interacting with backend device APIs (e.g. OpenMP, CUDA, OpenCL), uses just-in-time compilation to build backend kernel, and provide a kernel language, a minor extension to C, to abstract programming for each backend.

<https://libocca.org>

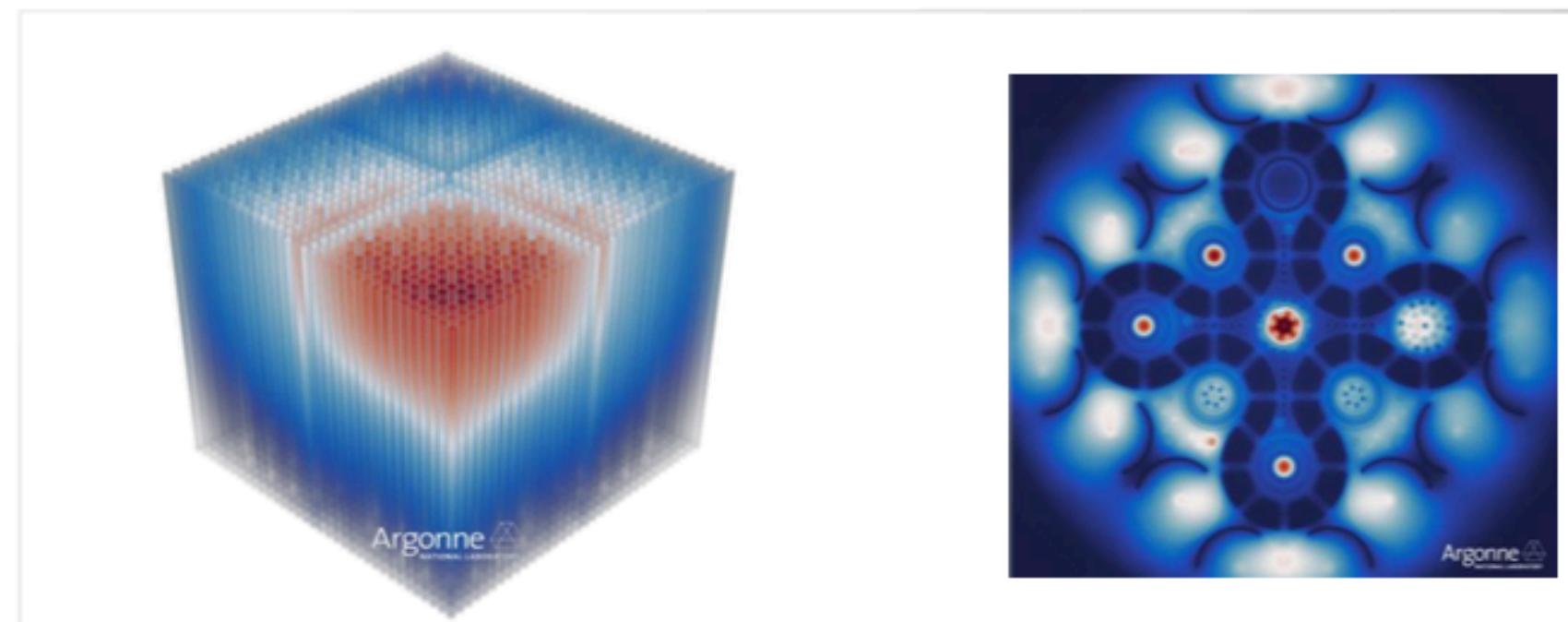
# Showcase

## ExaSMR: OpenMC Performance on Ponte Vecchio

Monte Carlo particle transport code for exascale computations

Ponte Vecchio with OpenMP Target offload

2x performance lead



Exascale Compute Project Annual Meeting 2022 presentation:

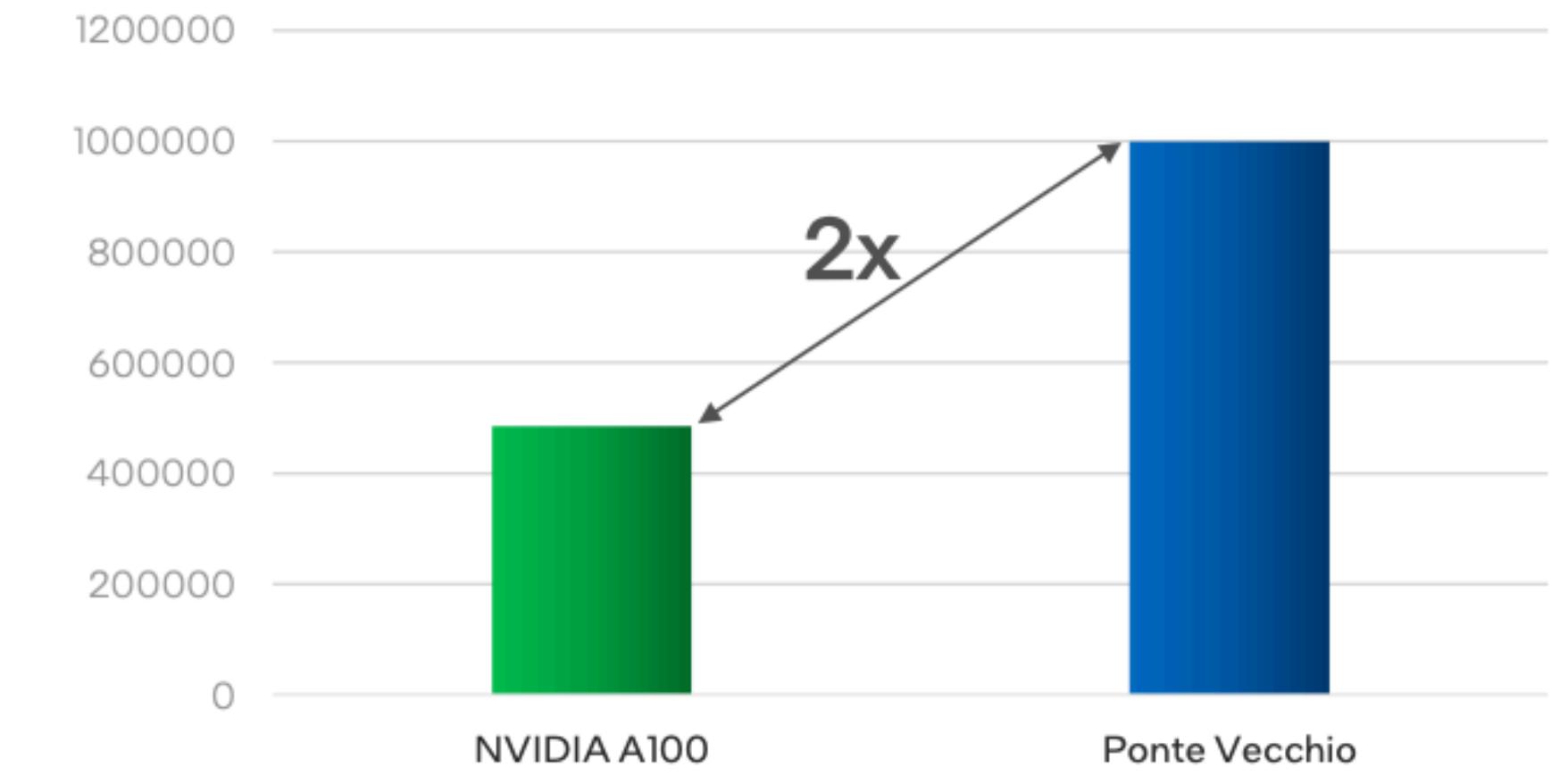
<https://www.alcf.anl.gov/events/2022-ecp-annual-meeting>

International Conference on Physics of Reactors 2022 presentation:

<https://www.ans.org/meetings/physor2022/session/view-976/>

<https://docs.openmc.org>

OpenMC Depleted Fuel Inactive Batch Performance  
on HM-Large Reactor with 40M particles  
(particles/second, Higher is better)



**Application Summary:** OpenMC is a Monte Carlo particle transport application that has recently been ported to the OpenMP target offloading programming model for use on GPU-based systems. The Monte Carlo method employed by OpenMC is considered the "gold standard" for high-fidelity simulation while also having the advantage of being a general-purpose method able to simulate nearly any geometry or material without the need for domain-specific assumptions. However, despite the extreme advantages in ease of use and accuracy, Monte Carlo methods like those in OpenMC often suffer from a very high computational cost. The extreme performance gains OpenMC has achieved on GPUs, as compared to traditional CPU architectures, is finally bringing within reach a much larger class of problems that historically were deemed too expensive to simulate using Monte Carlo methods. The leap in performance that GPUs are now offering carries with it the potential to disrupt a number of engineering technology stacks that have traditionally been dominated by non-general deterministic methods. For instance, faster MC applications may greatly expand the design space and simplify the regulation process for new nuclear reactor designs -- potentially improving the economics of nuclear energy and therefore helping to solve the world's climate crisis.



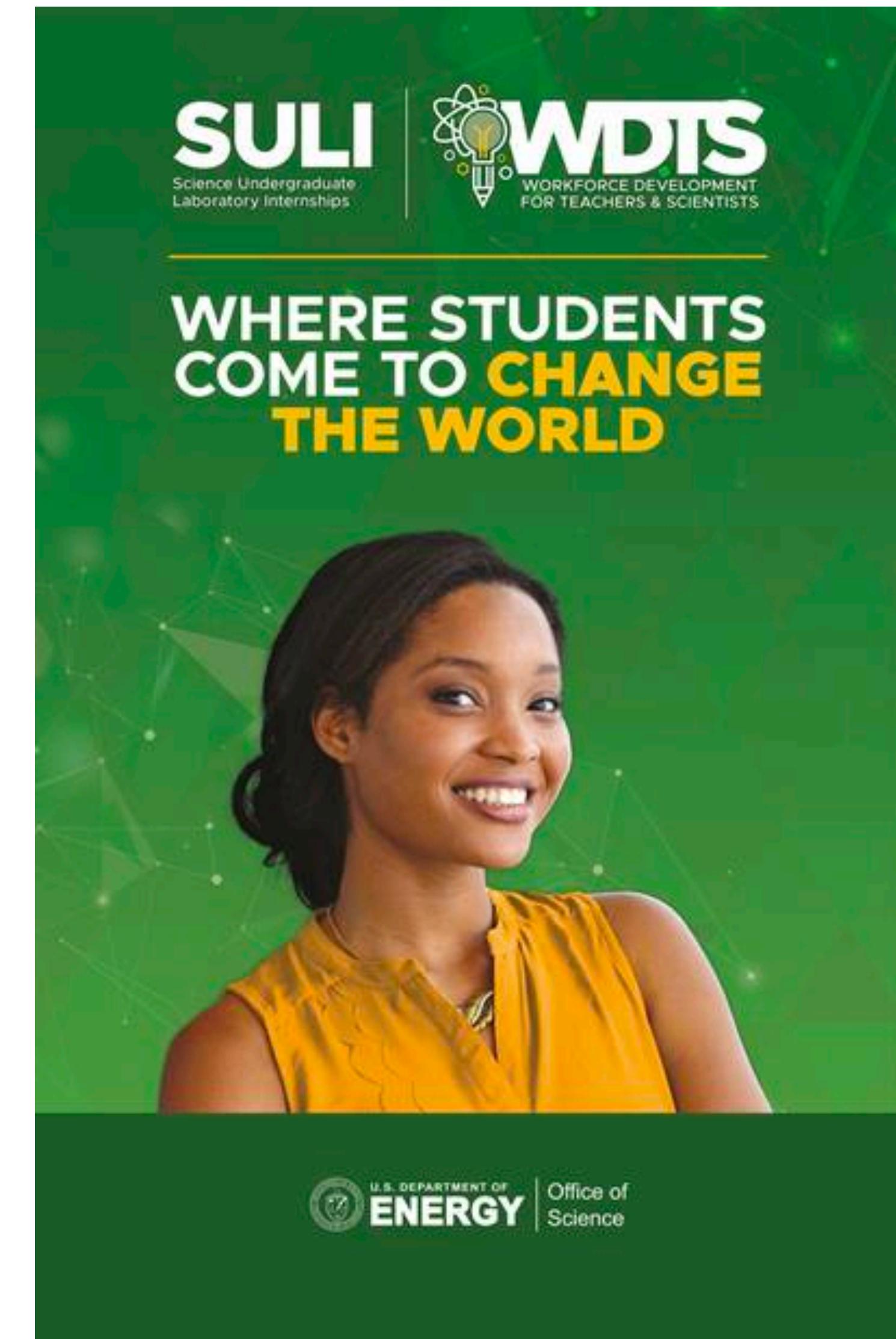
- See backup for workloads and configurations. Results may vary.
- Intel does not authorize the use of this material outside of Argonne National Laboratory. Downloaded on October 15, 2022 at 10:08:34 UTC from IEEE Xplore. Restrictions apply.



# Student Opportunities

- DOE's: [\*\*Science Undergraduate Laboratory Internship \(SULI\)\*\*](#)
  - Application:
    - How to Apply
    - open **NOW**
    - due **January 9, 2024**
- Argonne's: [\*\*Student Research Participation Program \(SRP\)\*\*](#)
  - Applications for Spring 2024 **NOW OPEN !!**
  - Deadline: **Friday, October 27, 2023**
- **Reach out!**

**APPLY NOW!!**



# Undergraduate Programs

- [Undergraduate Research Aide Program \(more info\)](#)
- [Community College Internship](#)
- [Professional Career Internship Program](#)
- [Minority Serving Institutions Partnership Program](#)
- [Lee Teng Undergrauate Fellowship in Accelerator Science](#)
- [Visiting Student Program for Undergraduate Students](#)
- [Seasonal Internship Program](#)
- [Sustainable Research Pathways \(SRP\)](#)

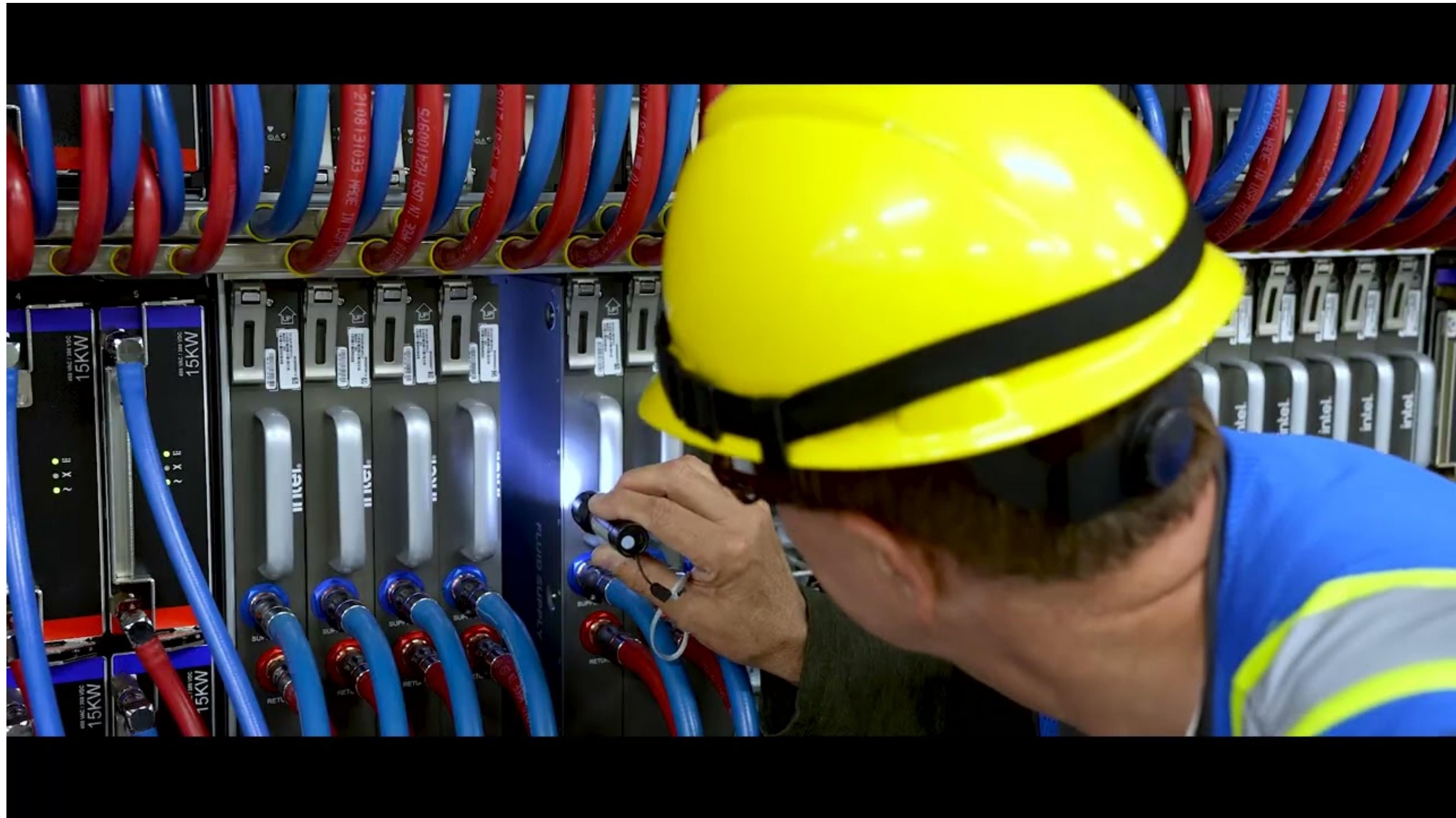
# Thank You!



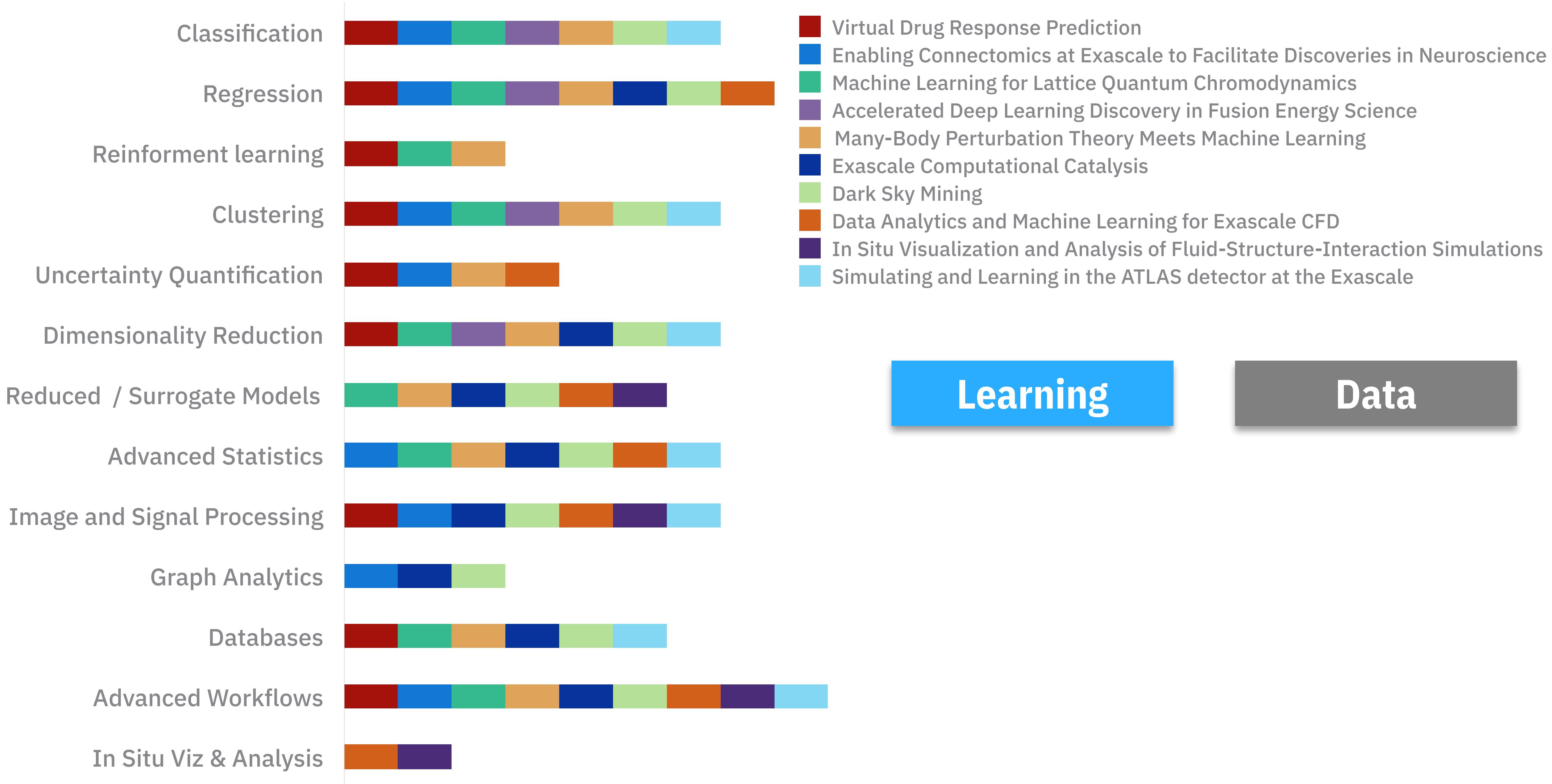
[foremans@anl.gov](mailto:foremans@anl.gov)

[@saforem2](https://twitter.com/saforem2)

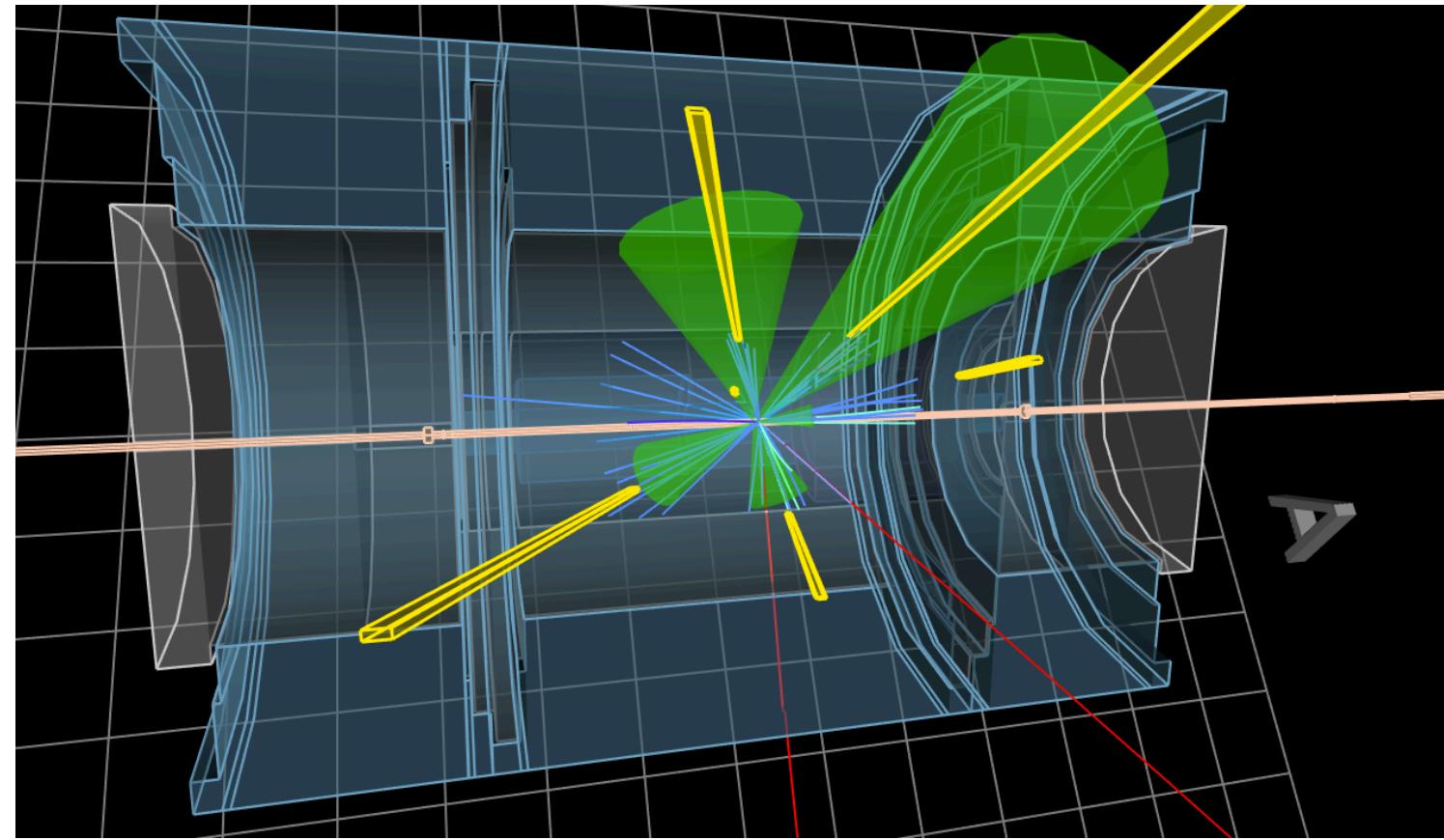
[samforeman.me](http://samforeman.me)



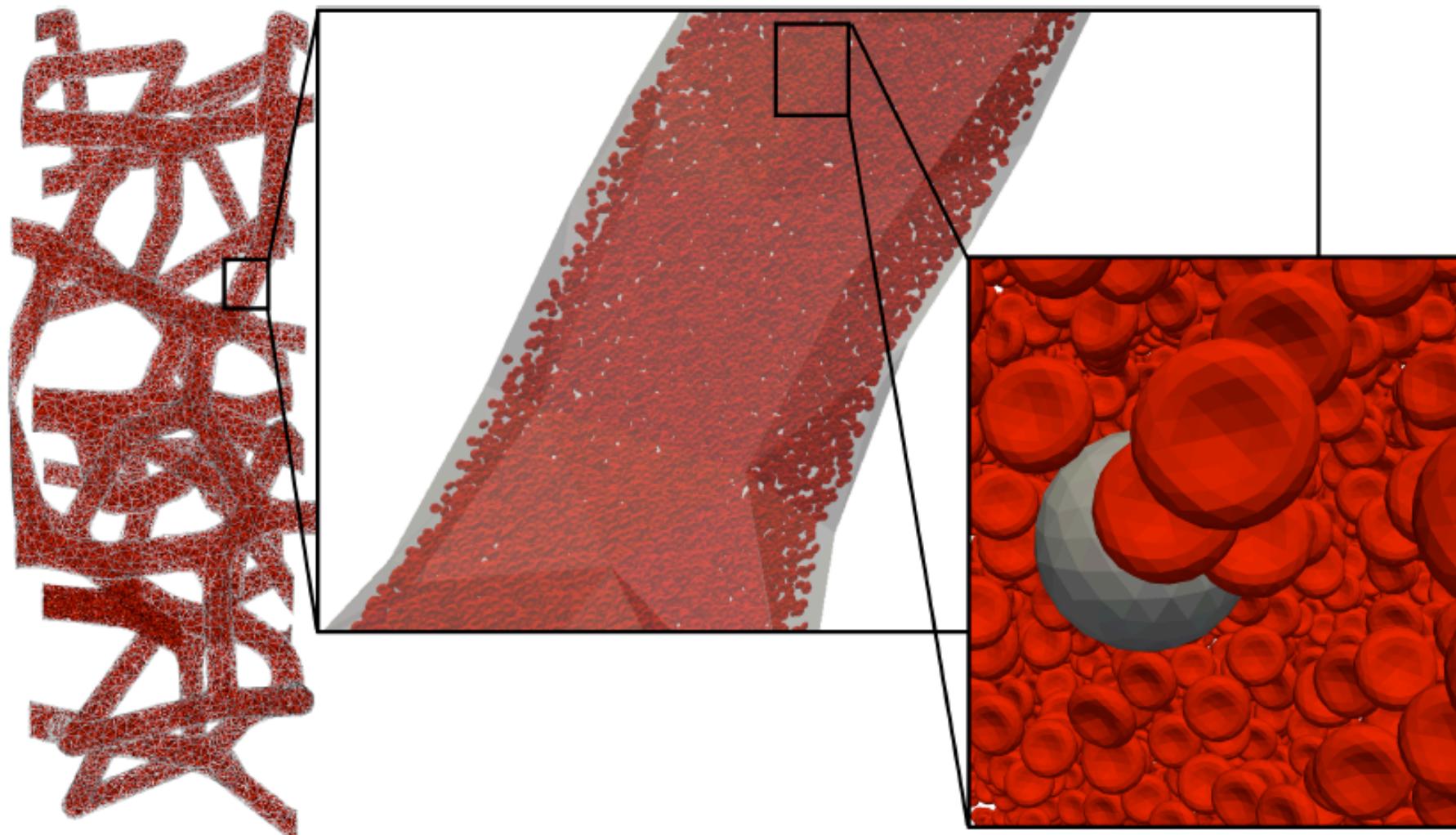
# AURORA ESP Data and Learning Projects and Methods



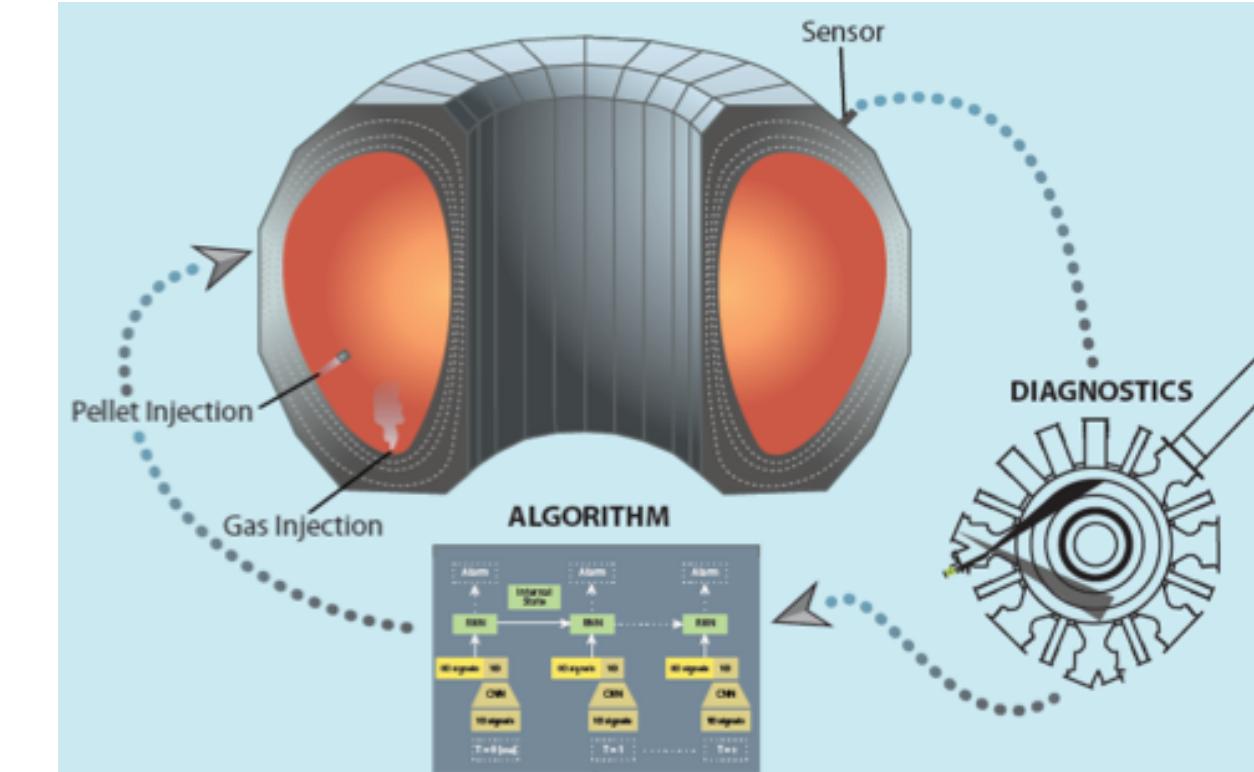
# Exascale Simulation, Data and Learning



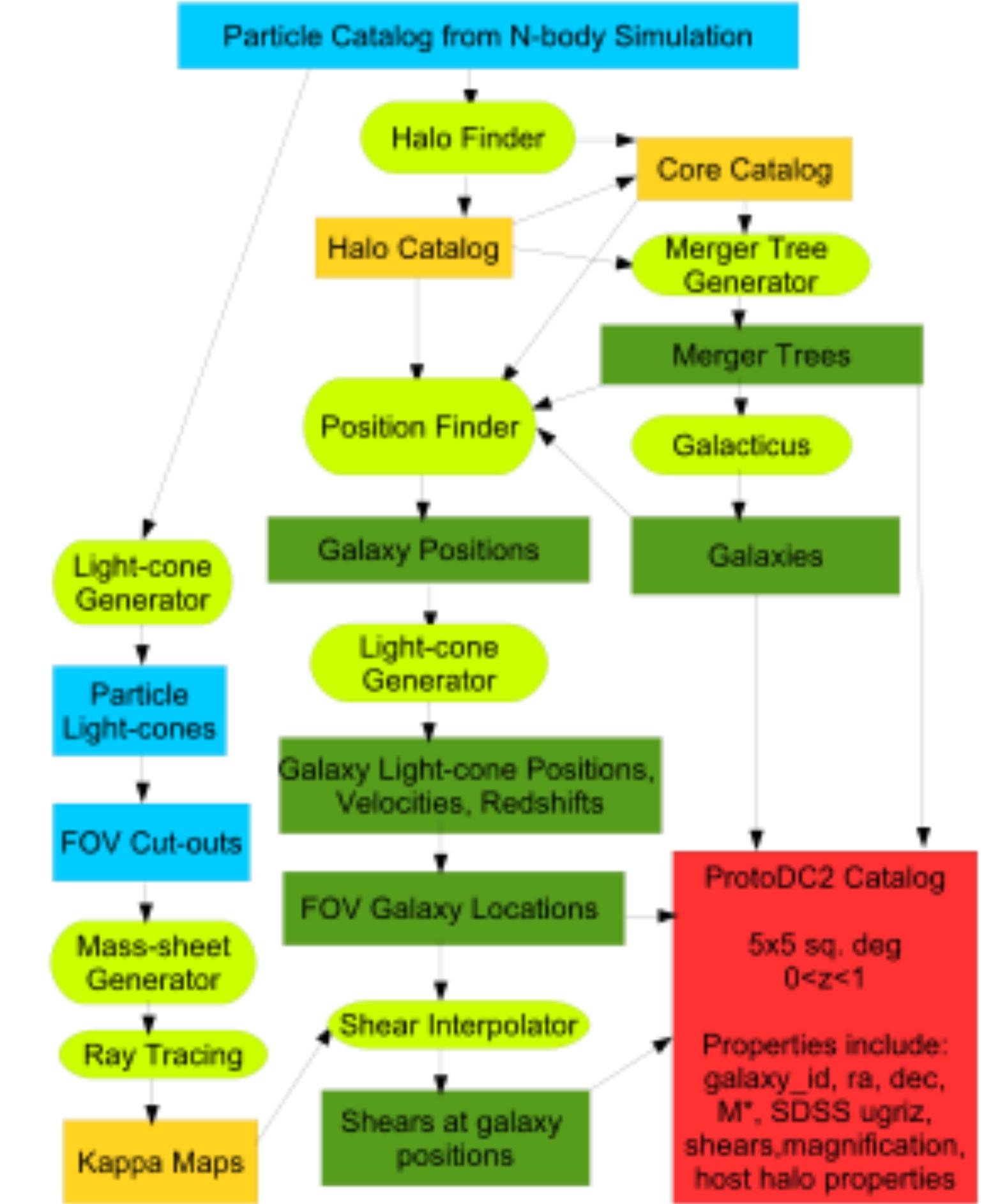
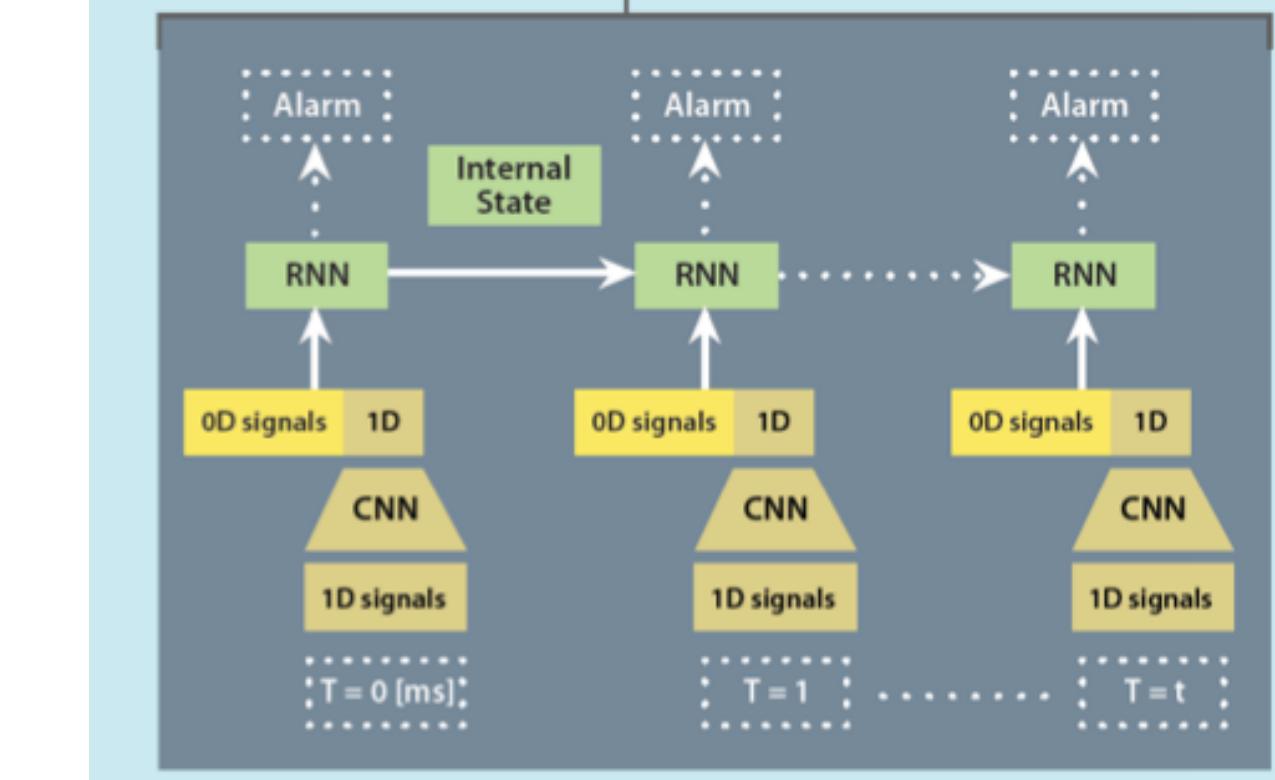
High Energy Physics



Bioscience, CFD



Fusion



Cosmology