Deploying and Operating Scientific Visualization Tools on HPC Systems

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September 26, 2025

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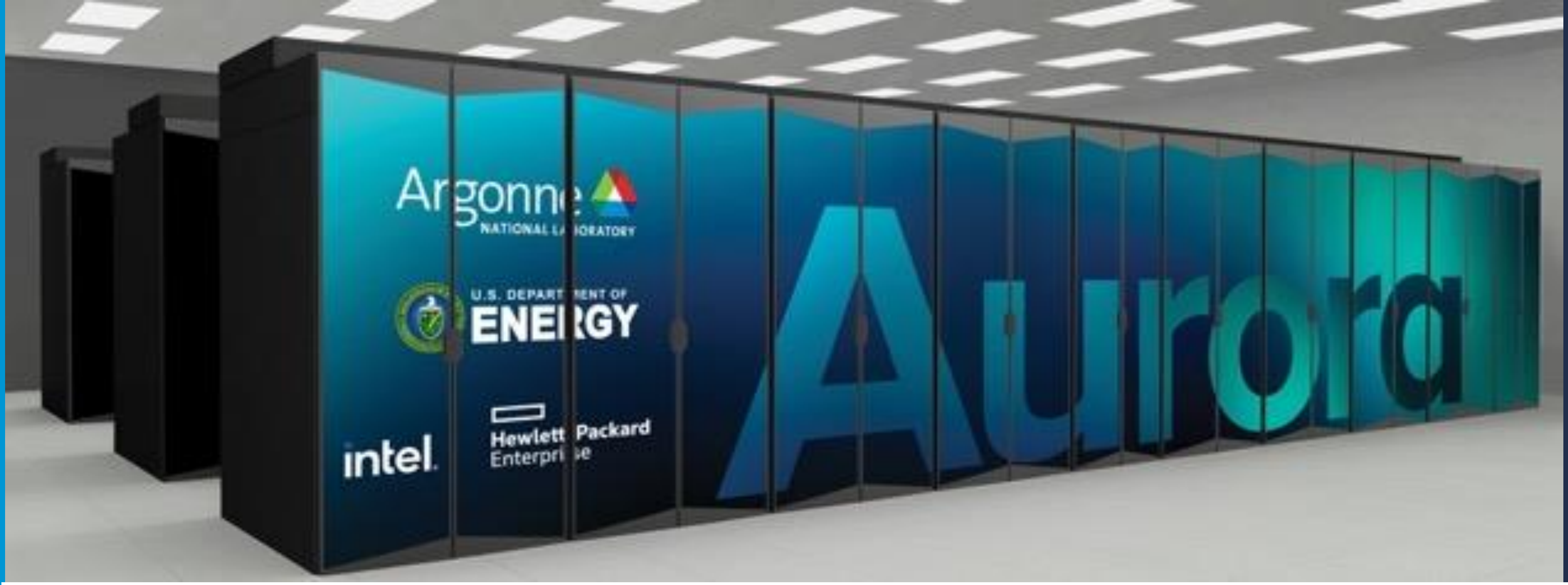

Aurora

Leadership Computing Facility Exascale Supercomputer

Peak Performance

≧ 2 Exaflops DP

Intel GPU

Intel® Data Center GPU Max Series

Intel Xeon Processor

4th Gen Intel XEON Max Series CPU

with High Bandwidth Memory

Platform

HPE Cray-Ex

Compute Node
Two 4th Gen Intel XEON Max Series CPUs
Six Intel® Data Center GPU Max Series
Node Unified Memory Architecture
Eight fabric endpoints

GPU Architecture
Intel® Data Center GPU Max Series architecture
High Bandwidth Memory Stacks

Node Performance
>130 TF

System Size
>10,000 nodes

Aggregate System Memory
>10 PB aggregate System Memory

System Interconnect
HPE Slingshot 11
Dragonfly topology with adaptive routing

Network Switch
25.6 Tb/s per switch (64 200 Gb/s ports)
Links with 25 GB/s per direction

High-Performance Storage
220 PB
≧25 TB/s DAOS bandwidth

Software Environment
- C/C++
- Fortran
- SYCL/DPC++
- OpenMP offload
- Kokkos
- RAJA
- Intel Performance Tools

Scientific Visualization on HPC Resources

- Visit and ParaView as open source tools
- Community efforts evolving for 20+ years
- Built on VTK (Visualization Toolkit)
- Viskores for acceleration

VTK Basics

- Provides common data models: polygonal data, points, image stacks, unstructured grids
- Parallel readers: read native simulation data and convert to VTK model
- Renderers: project data geometry into 2D images

DevOps Perspective: Visit and ParaView

- Complex applications with many dependencies
- Most building blocks are open source
- Domain decomposition: MPI ranks manage dataset chunks
- Final images assembled via compositing (collective MPI operations)

Rendering on a Supercomputer

- Headless rendering (no displays on compute nodes)
- OpenGL if available (requires X server context)
- OSMesa for CPU-based rendering (no GPU/driver)
- OSPRay ray tracing as an alternative (CPU-based)

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Building and Deploying: Overview

- Complex build systems
- *build_visit* (bash script) for Visit
- ParaView *superbuild* (CMake-based) for ParaView
- Automate retrieval and build of dependencies from source

Build Components

- CMake, Python, NumPy, SciPy, many Python libraries
- LLVM required for OSMesa
- VTK and Viskores for visualization algorithms
- Numerous parallel data readers
- Example: National labs (e.g., LANL) dedicate staff to maintain ParaView

Ingesting Data into Visit and ParaView

- Multiple data readers available
- Simulation data models may not map directly
- Example: Nek5000 spectral element data → needs conversion to unstructured grid → large data expansion

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Client/Server Mode: Workflow

- Most common interactive mode
- Client launches connection → login node → queued job on HPC
- Once running, parallel app reverse connects to client
- Typical chain: Client ↔ Login node ↔ Head compute node
- Tools like socat often needed for connection management

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QUESTIONS?

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