#### Present and Future Leadership Computers at OLCF

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



#### Oak Ridge Leadership Computing Facility (OLCF)

# Mission: Deploy and operate the computational resources required to tackle global challenges

- Providing world-leading computational and data resources and specialized services for the most computationally intensive problems
- Providing stable hardware/software path of increasing scale to maximize productive applications development
- Providing the resources to investigate otherwise inaccessible systems at every scale: from galaxy formation to supernovae to earth systems to automobiles to nanomaterials
- With our partners, deliver transforming discoveries in materials, biology, climate, energy technologies, and basic science

#### Our Science requires that we continue to advance OLCF's computational capability over the next decade on the roadmap to Exascale.

Since clock-rate scaling ended in 2003, HPC performance has been achieved through increased parallelism. Jaguar scaled to 300,000 cores. Titan and beyond deliver hierarchical parallelism with very powerful nodes. MPI plus thread level parallelism through OpenACC or OpenMP plus vectors



#### **Today's Leadership System - Titan** Hybrid CPU/GPU architecture, Hierarchical Parallelism

#### Vendors: Cray<sup>™</sup> / NVIDIA<sup>™</sup>

- 27 PF peak
- 18,688 Compute nodes, each with
  - 1.45 TF peak
  - NVIDIA Kepler™ GPU 1,311 GF
    - 6 GB GDDR5 memory
  - AMD Opteron<sup>™</sup>- 141 GF
    - 32 GB DDR3 memory
  - PCIe2 link between GPU and CPU
- Cray Gemini 3-D Torus Interconnect
- 32 PB / 1 TB/s Lustre<sup>®</sup> file system





### Where do we go from here?

 Provide the Leadership computing capabilities needed for the DOE Office of Science mission from 2018 through 2022

Capabilities for INCITE and ALCC science projects

- CORAL was formed by grouping the three Labs who would be acquiring Leadership computers in the same timeframe (2017).
  - Benefits include:
    - Shared technical expertise
    - Decreases risks due to the broader experiences, and broader range of expertise of the collaboration
    - Lower collective cost for developing and responding to RFP



## **CORAL** <u>Collaboration</u> <u>ORNL</u>, <u>ANL</u>, <u>LLNL</u>)

**Objective -** Procure 3 leadership computers to be sited at Argonne, Oak Ridge and Lawrence Livermore in 2017. Two of the contracts have been awarded with the Argonne contract in process.

#### Current DOE Leadership Computers

Titan (ORNL) 2012 - 2017 Sequoia (LLNL)

Mira (ANL) 2012 - 2017







**Leadership Computers** RFP requests >100 PF, 2 GB/core main memory, local NVRAM, and science performance 4x-8x Titan or Sequoia

#### Approach

- Competitive process one RFP (issued by LLNL) leading to 2 R&D contracts and 3 computer procurement contracts
- For risk reduction and to meet a broad set of requirements, 2 architectural paths will be selected and Oak Ridge and Argonne must choose different architectures
- Once Selected, Multi-year Lab-Awardee relationship to co-design computers
- Both R&D contracts jointly managed by the 3 Labs
- Each lab manages and negotiates its own computer procurement contract, and may exercise options to meet their specific needs
- Understanding that long procurement lead-time may impact architectural characteristics and designs of procured computers



### **Two Architecture Paths for Today and Future Leadership Systems**

Power concerns for large supercomputers are driving the largest systems to either Hybrid or Many-core architectures

#### Hybrid Multi-Core (like Titan)

- CPU / GPU hybrid systems
- Likely to have multiple CPUs and GPUs per node
- Small number of very powerful nodes
- Expect data movement issues to be much easier than previous systems – coherent shared memory within a node
- Multiple levels of memory on package, DDR, and non-volatile

#### Many Core (like Sequoia/Mira)

- 10's of thousands of nodes with millions of cores
- Homogeneous cores
- Multiple levels of memory on package, DDR, and non-volatile
- Unlike prior generations, future products are likely to be self hosted



### 2017 OLCF Leadership System Hybrid CPU/GPU architecture



At least 5X Titan's Application Performance

Approximately 3,400 nodes, each with:

- Multiple IBM POWER9 CPUs and multiple NVIDIA Tesla® GPUs using the NVIDIA Volta architecture
- CPUs and GPUs completely connected with high speed NVLink
- Large coherent memory: over 512 GB (HBM + DDR4)
  - all directly addressable from the CPUs and GPUs
- An additional 800 GB of NVRAM, which can be configured as either a burst buffer or as extended memory
- over 40 TF peak performance

Dual-rail Mellanox<sup>®</sup> EDR-IB full, non-blocking fat-tree interconnect

IBM Elastic Storage (GPFS<sup>™</sup>) - 1TB/s I/O and 120 PB disk capacity.





#### **INTRODUCING NVLINK AND HBM MEMORY** TRANSFORMATIVE TECHNOLOGY FOR 2016 WITH POWER 8+<sup>®</sup>, AND BEYOND

#### NVLINK

GPU high speed interconnect
5X-12X PCI-E Gen3 Bandwidth
Planned support for POWER<sup>®</sup> CPUs



- 4x Higher Bandwidth (~1 TB/s)
- 3x Larger Capacity
- 4x More Energy Efficient per bit







9 <mark>@ NVIDIA</mark>.

#### Summit's High-Speed Interconnect Mellanox Technologies® Dual-Rail EDR Infiniband

#### InfiniBand Interconnect Three-level Fat Tree Interconnect

- 3-Level Fat Tree
- 23 GB/s (dual plane 100Gb/s)
- 5 hops max
- Adaptive routing





### **Summit Key Software Components**

#### System

- Linux®
- IBM Elastic Storage (GPFS<sup>™</sup>)
- IBM Platform Computing<sup>™</sup> (LSF)
- IBM Platform Cluster Manager<sup>™</sup> (xCAT)

#### Programming Environment

- Compilers supporting OpenMP and OpenACC
  - IBM XL, PGI, LLVM, GNU, NVIDIA
- Libraries
  - IBM Engineering and Scientific Subroutine Library (ESSL)
  - FFTW, ScaLAPACK, PETSc, Trilinos, BLAS-1,-2,-3, NVBLAS
  - cuFFT, cuSPARSE, cuRAND, NPP, Thrust
- Debugging
  - Allinea DDT, IBM Parallel Environment Runtime Edition (pdb)
  - Cuda-gdb, Cuda-memcheck, valgrind, memcheck, helgrind, stacktrace
- Profiling
  - IBM Parallel Environment Developer Edition (HPC Toolkit)
  - VAMPIR, Tau, Open|Speedshop, nvprof, gprof, Rice HPCToolkit



### How does Summit compare to Titan

Feature	Summit	Titan
Application Performance	5-10x Titan	Baseline
Number of Nodes	~3,400	18,688
Node performance	> 40 TF	1.4 TF
Memory per Node	>512 GB (HBM + DDR4)	38GB (GDDR5+DDR3)
NVRAM per Node	800 GB	0
Node Interconnect	NVLink (5-12x PCIe 3)	PCIe 2
System Interconnect (node injection bandwidth)	Dual Rail EDR-IB (23 GB/s)	Gemini (6.4 GB/s)
Interconnect Topology	Non-blocking Fat Tree	3D Torus
Processors	IBM POWER9 NVIDIA Volta™	AMD Opteron™ NVIDIA Kepler™
File System	120 PB, 1 TB/s, GPFS™	32 PB, 1 TB/s, Lustre <sup>®</sup>
Peak power consumption	10 MW	9 MW



# **Questions?**





#### **U.S. DEPARTMENT OF ENERGY** Office of Science

#### GPU Hackathon October 2014

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