Enabling large scale science on Summit with highly efficient scientific applications developed through the Center for Accelerated Application Readiness

Tjerk Straatsma and Jack C. Wells
Oak Ridge Leadership Computing Facility
Oak Ridge National Laboratory

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What is a Leadership Computing Facility (LCF)?

- Collaborative DOE Office of Science user-facility program at ORNL and ANL
- Mission: Provide the computational and data resources required to solve the most challenging problems.
- 2-centers/2-architectures to address diverse and growing computational needs of the scientific community
- Highly competitive user allocation programs (INCITE, ALCC).
- Projects receive 10x to 100x more resource than at other generally available centers.
- LCF centers partner with users to enable science & engineering breakthroughs (Liaisons, Catalysts).
ORNL has systematically delivered a series of leadership-class systems
On scope • On budget • Within schedule

Titan, five years old in October 2017, continues to deliver world-class science research in support of our user community. We will operate Titan through 2019 when it will be decommissioned.
We are building on this record of success to enable exascale in 2021.

- Titan (2012, Cray XK7) with 27 PF
- Summit (2018, IBM) with 200 PF
- OLCF-4
- OLCF-5
- Frontier (2021) with ~1 EF

500-fold improvement in 9 years.
Coming in 2018: Summit will replace Titan as the OLCF’s leadership supercomputer

Summit, slated to be more powerful than any other existing supercomputer, is the Department of Energy’s Oak Ridge National Laboratory’s newest supercomputer for open science.
Summit Overview

Components
IBM POWER9
- 22 Cores
- 4 Threads/core
- NVLink

2 x POWER9
6 x NVIDIA GV100
NVMe-compatible PCIe 1600 GB SSD

Compute Rack
18 Compute Servers
Warm water (70°F direct-cooled components)
RDHX for air-cooled components

25 GB/s EDR IB (2 ports)
512 GB DRAM (DDR4)
96 GB HBM (3D Stacked)
Coherent Shared Memory

39.7 TB Memory/rack
55 KW max power/rack

Compute System
10.2 PB Total Memory
256 compute racks
4,608 compute nodes
Mellanox EDR IB fabric
200 PFLOPS
~13 MW

GPFS File System
250 PB storage
2.5 TB/s read, 2.5 TB/s write
Summit Node Overview

- **TF**: 42 TF (6x7 TF)
- **HBM**: 96 GB (6x16 GB)
- **DRAM**: 512 GB (2x16x16 GB)
- **NET**: 25 GB/s (2x12.5 GB/s)
- **MMs/s**: 83

HBM & DRAM speeds are aggregate (Read+Write). All other speeds (X-Bus, NVLink, PCIe, IB) are bi-directional.

HBM/DRAM Bus (aggregate B/W)
- NVLink
- X-Bus (SMP)
- PCIe Gen4
- EDR IB

HBM & DRAM speeds are aggregate (Read+Write). All other speeds (X-Bus, NVLink, PCIe, IB) are bi-directional.
IBM Power9 Processor

• Up to 24 cores
  – CORAL has 22 cores for yield optimization on first processors

• PCI-Express 4.0
  – Twice as fast as PCIe 3.0

• NVLink 2.0
  – Coherent, high-bandwidth links to GPUs

• 14nm FinFET SOI technology
  – 8 billion transistors

• Cache
  – L1I: 32 KiB per core, 8-way set associative
  – L1D: 32KiB per core, 8-way
  – L2: 258 KiB per core
  – L3: 120 MiB eDRAM, 20-way
Volta Details

<table>
<thead>
<tr>
<th>PERFORMANCE with NVIDIA GPU Boost&lt;sup&gt;®&lt;/sup&gt;</th>
<th>Tesla V100 for NVLink</th>
<th>Tesla V100 for PCIe</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOUBLE-PRECISION</td>
<td>7.8 TeraFLOPS</td>
<td>7 TeraFLOPS</td>
</tr>
<tr>
<td>SINGLE-PRECISION</td>
<td>15.7 TeraFLOPS</td>
<td>14 TeraFLOPS</td>
</tr>
<tr>
<td>DEEP LEARNING</td>
<td>125 TeraFLOPS</td>
<td>112 TeraFLOPS</td>
</tr>
</tbody>
</table>

| INTERCONNECT BANDWIDTH Bi-Directional       | NVLINK 300 GB/s       | PCIE 32 GB/s        |

<table>
<thead>
<tr>
<th>MEMORY CoWoS Stacked HBM2</th>
<th>CAPACITY 16 GB HBM2</th>
</tr>
</thead>
<tbody>
<tr>
<td>BANDWIDTH</td>
<td>900 GB/s</td>
</tr>
</tbody>
</table>

Note: The performance numbers are peak and not representative of Summit’s Volta
Coming in 2018: Summit will replace Titan as the OLCF’s leadership supercomputer

- Many fewer nodes
- Much more powerful nodes
- Much more memory per node and total system memory
- Faster interconnect
- Much higher bandwidth between CPUs and GPUs
- Much larger and faster file system

<table>
<thead>
<tr>
<th>Feature</th>
<th>Titan</th>
<th>Summit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Application Performance</td>
<td>Baseline</td>
<td>5-10x Titan</td>
</tr>
<tr>
<td>Number of Nodes</td>
<td>18,688</td>
<td>4,608</td>
</tr>
<tr>
<td>Node performance</td>
<td>1.4 TF</td>
<td>42 TF</td>
</tr>
<tr>
<td>Memory per Node</td>
<td>32 GB DDR3 + 6 GB GDDR5</td>
<td>512 GB DDR4 + 96 GB HBM2</td>
</tr>
<tr>
<td>NV memory per Node</td>
<td>0</td>
<td>1600 GB</td>
</tr>
<tr>
<td>Total System Memory</td>
<td>710 TB</td>
<td>&gt;10 PB DDR4 + HBM2 + Non-volatile</td>
</tr>
<tr>
<td>System Interconnect</td>
<td>Gemini (6.4 GB/s)</td>
<td>Dual Rail EDR-IB (25 GB/s)</td>
</tr>
<tr>
<td>Interconnect Topology</td>
<td>3D Torus</td>
<td>Non-blocking Fat Tree</td>
</tr>
<tr>
<td>Bi-Section Bandwidth</td>
<td>15.6 TB/s</td>
<td>115.2 TB/s</td>
</tr>
<tr>
<td>Processors</td>
<td>1 AMD Opteron™</td>
<td>2 IBM POWER9™</td>
</tr>
<tr>
<td></td>
<td>1 NVIDIA Kepler™</td>
<td>6 NVIDIA Volta™</td>
</tr>
<tr>
<td>File System</td>
<td>32 PB, 1 TB/s, Lustre®</td>
<td>250 PB, 2.5 TB/s, GPFS™</td>
</tr>
<tr>
<td>Power Consumption</td>
<td>9 MW</td>
<td>13 MW</td>
</tr>
</tbody>
</table>
What is CORAL?
The program through which Summit & Sierra are procured.

- Several DOE labs have strong supercomputing programs and facilities.
- To bring the next generation of leading supercomputers to these labs, DOE created CORAL (the Collaboration of Oak Ridge, Argonne, and Livermore) to jointly procure these systems, and in so doing, align strategy and resources across the DOE enterprise.
- Collaboration grouping of DOE labs was done based on common acquisition timings. Collaboration is a win-win for all parties.

OpenPOWER Technologies: IBM POWER CPUs, NVIDIA Tesla GPUs, Mellanox EDR 100Gb/s InfiniBand

Paving The Road to Exascale Performance
OLCF Program to Ready Application Developers and Users

• We are preparing users through:
  – Application Readiness and Early Science through Center for Accelerated Application Readiness (CAAR)
  – Training and web-based documentation
  – Early access on SummitDev and Summit Phase I system (already accepted)
  – Access for broader user base on final, accepted Phase II system

• Goals:
  – Early science achievements,
  – Demonstrate application readiness,
  – Prepare INCITE & ALCC proposals,
  – Harden Summit for full-user operations
Center for Accelerated Application Readiness (CAAR) Projects
2015 - 2018

**ACME:** Climate Research: Advancing Earth System Models  
Pl: Dr. David Bader, Lawrence Livermore National Laboratory  
Science Domain: Climate Science  
CAAR Liaison: Dr. Matt Norman  
CSEEN Postdoc: Dr. Anikesh Pal  
NESAP

**DIRAC:** CAAR Oak Ridge Proposal for getting the Relativistic Quantum Chemistry Program Package DIRAC ready for SUMMIT  
Pl: Prof. Dr. Lucas Visscher, Free University Amsterdam, the Netherlands  
Science Domain: Relativistic Quantum Chemistry  
CAAR Liaisons: Dr. Dmitry Liakh, Dr. Tjerk Straatsma  
CSEEN Postdoc: TBD (backfill Dr. Amelia Fitzsimmons)

**FLASH:** Using FLASH for Astrophysics Simulations at an Unprecedented Scale  
Pl: Dr. Bronson Messer, Oak Ridge National Laboratory  
Science Domain: Astrophysics  
CAAR Liaisons: Dr. Bronson Messer  
CSEEN Postdoc: Dr. Austin Harris

**GTC:** Particle Turbulence Simulations for Sustainable Fusion Reactions in ITER  
Pl: Prof. Dr. Zhihong Lin, University of California - Irvine  
Science Domain: Plasma Physics  
CAAR Liaison: Dr. Wayne Joubert  
NESAP

**HACC:** Cosmological Simulations for Large-scale Sky Surveys  
Pl: Dr. Salman Habib, Argonne National Laboratory  
Science Domain: Cosmology  
CAAR Liaison: Dr. Bronson Messer  
NESAP, ESP

**LS-DALTON:** Large-scale Coupled-cluster Calculations of Supramolecular Wires  
Pl: Prof. Dr. Poul Jørgensen, Aarhus University  
Science Domain: Quantum Chemistry  
CAAR Liaison: Dr. Dmytro Bykov  
INCITE

**RATOR:** Fluid Dynamics Research to Accelerate Combustion Science  
Pl: Dr. Joseph Oefelein, Sandia National Laboratory, Livermore  
Science Domain: Engineering/Combustion  
CAAR Liaison: Dr. Ramanan Sankaran  
CSEEN Postdoc: TBD (backfill Dr. Kalyana Gottiparthi)

**NAMD:** Molecular Machinery of the Brain  
Pl: Dr. James Phillips, University of Illinois at Urbana-Champaign  
Science Domain: Biophysics  
CAAR Liaison: Dr. Tjerk Straatsma  
NESAP

**NUCCOR:** Nuclear Structure and Nuclear Reactions  
Pl: Dr. Gaute Hagen, Oak Ridge National Laboratory  
Science Domain: Nuclear Physics  
CAAR Liaison: Dr. Gustav Jansen  
CSEEN Postdoc: TBD (backfill Dr. Micah Schuster)

**NWChem:** Developing Coupled Cluster Methodologies for GPUs  
Pl: Dr. Paul R. C. Kent, Oak Ridge National Laboratory  
Science Domain: Materials Science  
CAAR Liaison: Dr. Ying Wai Li  
CSEEN Postdoc: Dr. Andreas Tillack

**QMCPACK:** Materials Science Research for High-Temperature Superconductors  
Pl: Dr. Karol Kowalski, Pacific Northwest National Laboratory  
Science Domain: Computational Chemistry  
CAAR Liaison: Dr. Dmitry Liakh  
IBM Postdoc: Dr. David Appelhans  
NESAP

**SPECFEM:** Mapping the Earth’s Interior Using Big Data  
Pl: Dr. Jeroen Tromp, Princeton University, Princeton University  
Science Domain: Seismology  
CAAR Liaison: Dr. Judy Hill  
CSEEN Postdoc: Dr. Yangkang Chen

**XGC:** Multiphysics Magnetic Fusion Reactor Simulator, from Hot Core to Cold Wall  
Pl: Dr. CS Chang, Princeton Plasma Physics Laboratory, Princeton University  
Science Domain: Plasma Physics  
CAAR Liaison: Dr. Ed D’Azevedo  
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**NESAP**
SummitDev Early Access System

Each IBM S822LC node has:
- 2x IBM POWER8+ CPUs
  - 32x 8GB DDR4 memory (256 GB)
  - 10 cores per POWER8+, each core with 8 HW threads
- 4x NVIDIA Tesla P100 GPUs
  - NVLink 1.0 connects GPUs at 80 GB/s
  - 16 GB HBM2 memory per GPU
- 2x Mellanox EDR InfiniBand
- 1600 GB NVMe storage

Summit Early Access System:
- 3 racks for development, each with 18 nodes
- One rack of login and support servers
- Nodes connected in a full fat-tree via EDR InfiniBand
- Liquid cooled w/ heat exchanger rack
- One additional 18-node rack is for system software testing
- Primary purpose is for code teams to prepare applications for Summit
Research supported by the DOE SC/NP seeks to understand the nuclear processes that have shaped the cosmos, including the origin of the elements, the evolution of stars, and the detonation of supernovae.

FLASH is a publicly available, component-based, massively parallel, adaptive mesh refinement (AMR) code that has been used on a variety of parallel platforms.

In particular, measurements made at the under-construction Facility for Rare Isotope Beams (FRIB) – coupled with simulations of the late-time evolution of supernovae – will help determine how the elements from iron to uranium are created.

Targeted for CAAR

1. Hydrodynamics module performance
2. Equation of State (EOS) threading and vectorization
3. Nuclear kinetics (burn unit) threading and vectorization, including Jacobian formation and solution using GPU-enabled libraries

http://flash.uchicago.edu
FLASH Early Summit Results

- FLASH: Component-based, massively parallel, adaptive-mesh refinement code
  - Widely used in astrophysics community (>1100 publications from >600 scientists)
- CAAR work primarily concerned with increasing physical fidelity by accelerating the nuclear burning module and associated load balancing.
- Summit GPU performance **fundamentally changes the potential science impact** by enabling large-network (i.e. 160 or more nuclear species) simulations.
  - Heaviest elements in the Universe are made in neutron-rich environments – small networks are incapable of tracking these neutron-rich nuclei
  - Opens up the possibility of producing precision nucleosynthesis predictions to compare to observations
  - Provides detailed information regarding most astrophysically important nuclear reactions to be measured at FRIB

Preliminary results on Summit

**GPU+CPU vs. CPU-only performance on Summit for 288-species network:** 2.9x

P9: 24.65 seconds/step

**P9 + Volta:** 8.5 seconds/step

**288-species impossible to run on Titan**

Bronson Messer, J. Austin Harris, Tom Papatheodore (ORNL)
QMCPACK is an open source, ab initio quantum Monte Carlo code for the study and prediction of materials properties by stochastically solving quantum many-body problems using variational MC and more accurate but computationally demanding diffusion MC. It allows for highly accurate, predictive ab initio calculations of larger and more complex systems that are limited or inaccessible by conventional methods such as density functional theory (DFT).

Algorithmic improvements and enhanced predictive capacity targeted by CAAR will accelerate the understanding of a wide range of materials, e.g., strongly correlated systems and transition elements, which are essential for materials design for energy capture, storage and conversion, as well as high temperature superconductors.

Targeted for CAAR:
1. Orbital evaluation and memory usage
2. Slater determinant evaluation: improve numerical stability of current (less computationally intensive) updating scheme
3. QMC energy evaluation: optimize and explore extra level(s) of parallelism to improve time-to-solution ratio
4. Load balancing: reduce synchronizations and global collection operations to maximize performance

http://qmcpack.org/
QMCPACK Early Summit Results

- QMCPACK: Accurate quantum mechanics-based simulation of materials, including high-temperature superconductors.
- QMCPACK runs correctly and with good initial performance on up to 64 Summit nodes.
- Runs use the latest version from GitHub without modification.
- Improvements to both Power CPU and Volta GPU performance are expected via optimization and new algorithms.
- A Summit node is 50-times faster than a Titan node for this problem, indicating a $\sim 3.7x$ increase in the complexity of materials (electron count) computable in the same wall time as Titan.

Paul Kent, Andreas Tillack, Ying Wai Li  (ORNL)
Domain Area: Astrophysics

Research motivated by the Cosmic Frontier Science Driver supported by the DOE Office of Science Program in High Energy Physics seeks to reveal the nature of dark matter and dark energy. The ancient light from distant galaxies allows the distribution of dark matter to be mapped and perhaps the nature of dark energy to be unraveled. Large-scale cosmological simulation is an essential tool in these investigations.

HACC is a particle-mesh cosmology code. It has been used to produce numerical surveys to guide the design of observational galaxy surveys and to develop prediction tools to help survey teams interpret large amounts of observational data.

Targeted for CAAR
1. The addition of baryonic hydrodynamics via Conservative Reproducing Kernel Smooth Particle Hydrodynamics (CRKSPH)
2. Optimization of both the Tree-PM and P^3M short-range solver on Summit
3. A new, GPU-enabled visualization and analysis framework

ECP ExaSky Project: First HACC Runs on Summit under CAAR Application Readiness

The HACC (Hardware/Hybrid Accelerated Cosmology Code) is being developed under ASCR’s Exascale Computing Project to carry out simulations for next-generation cosmological surveys sponsored by DOE HEP.

Matter distribution in the universe from a HACC test run on Summit at ORNL; this work is part of an OLCF Center for Accelerated Application Readiness (CAAR) supported project.

Demonstration of GPU acceleration on Summit with ExaSky’s extreme-scale HACC simulation framework.
Domain Area: Plasma Physics

Plasma Physics is a DOE/FES research program focused on advance research on magnetically confined plasmas to develop the science needed to create a sustainable fusion energy source.

XGC is a widely used advanced whole-device tokamak gyrokinetic code for modeling edge plasma at first-principles level. XGC is a 5D gyrokinetic particle-in-cell (PIC) with finite element that can model tokamak plasma in realistic divertor magnetic geometry with neutral particle recycling at material wall surface.

Whole device integrated modeling for ITER to obtain understanding of the edge pedestal boundary physics and disruption events are Tier 1 priority recommendation from DOE Fusion Energy Science Advisory Committee. Acceleration via the CAAR effort will greatly improve XGC’s ability to model these critical areas of interest.

Targeted for CAAR:
- Acceleration of computational kernels (particle push, collision physics, charge deposition) for GPU.
- Innovative use of NVRAM for check-point/restart, in-situ data analysis and data reduction.
- Reorganization of data structures to take advantage of deep memory hierarchies.

http://epsi.pppl.gov/computing/xgc-1
XGC Current Status

• Extended weak scaling to 1024 nodes for the GPU+CPU runs for the collisionless turbulence case, achieved a speedup of 7x.

• With collisions, the GPU-accelerated code [(CPU+GPU)/CPU] has a speedup of almost 9x.
Summit Early Science Program

1. Call for Proposals
   a. To be issued December 2017
   b. Open to CAAR teams and others who ported applications for Summit
   c. Rolling acceptance with a deadline in CY18Q2

2. Criteria
   a. Meeting CAAR scalability and performance targets
   b. Mission relevant scientific campaign

3. Goals
   a. Science achievements and publications early
   b. Demonstration of CAAR and other applications
   c. Transition of applications & projects to INCITE and/or ALCC programs
   d. Harden system for production and availability using important, mission-relevant applications
Summit Early Science Program (ESP)

- We put out a Call for Proposals in December 2017
  - Resulted in 62 Letters of Intent (LOI) received by year’s end.
    - 27 are from PIs at universities
    - 32 are from PIs at national laboratories or research institutions (DOE, NASA)
    - 14 are CAAR project-related LOIs
    - 27 have had past INCITE allocations
    - 9 have had past ALCC allocations
    - 15 have connections to the US DOE Exascale Computing Project
    - 9 are AI or deep learning-related
  - Proposals are due at the beginning of June
  - ESP Users will gain full access to Summit for early science later this year
Summit is still under construction

• We expect to accept the machine in Summer of 2018, allow early users on this year, and allocate our first users through the INCITE program in January 2019.

• We are continuing node and file storage installation and software testing.
Acknowledgment

• CAAR Principle Investigators and their teams: David Bader (ACME), Lucas Visscher (DIRAC), Zhihong Lin (GTC), Salman Habib (HACC), Poul Jørgensen (LSDALTON), Jim Phillips (NAMD), Gaute Hagen (NUCCOR), Karol Kowalski (NWCHEM), Paul Kent (QMCPACK), Joe Oefelein (RAPTOR), Jeroen Tromp (SPECFEM), and CS Chang (XGC)

• Director Discretionary Project CHM120 (COIN): Remco Havenith and Ria Broer

• Scientific Computing Staff: Matt Norman, Dmitry Liakh, Bronson Messer, Wayne Joubert, Dmytro Bykov, Gustav Jansen, Ying Wai Li, Ramanan Sankaran, Judy Hill, and Ed D’Azevedo

• CSEEN postdocs: Anikesh Pal, Amelia Fitzsimmons, Thom Papatheodore, Austin Harris, Micah Schuster, Andreas Tillack, Kalyana Gottiparthi, Yangkang Chen, and Stephen Abbott

• Center of Excellence Staff: Eric Luo, Matt Niemerg, Jeff Larkin, and others

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Questions?
Jack Wells
wellsjc@ornl.gov