Updates from the OLCF

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OLCF User Group Meeting
Oak Ridge
15 May 2018

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Overview of Today’s Agenda

- OLCF Staff will give you a few Facility Updates
- Invited talks from OLCF Users Brant Robertson, Evan Schneider, Dan Jacobson, Wayne Joubert, P.K Yeung, and Matthew Clay.
- Two poster slam sessions at 10:30 am and 1:45 pm for our poster participants to briefly introduce their poster
- Lunch will be served next door, and we will have OLCF staff at each table to facilitate a discussion on a specific topic which will be noted on the table (outlined on next slide)
- We will take a Group Photo at 4:30
- There will be a voluntary tour of the OLCF and EVEREST facilities at 4:45 pm. For those interested, OLCF staff will escort you to the facilities.
- The poster session will take place out in the lobby from 5:15-6:30.
Round Table Lunch Topics

Tuesday Line-Up

• User Software Containers
• Tell your Story
• Continuous Integration
• OLCF Allocation Programs
• Constellation
• Employment Opportunities at the OLCF
• OLCF Website Feedback
• Performance Portability
• Deep Learning
• Center Management

Wednesday Line-Up

• Summit Early Science Program
• Data Initiatives/Programs
• Summit Burst Buffers
• OLCF Training
• JSRUN & LSF Tools on Summit
• Using Kokkos
• Software Engineering
• Machine Learning for Applications
• Analytics/Learning
Safety

- Emergency exits – There are two stair cases available in the case of an emergency.
- Please stop and listen if a safety announcement comes over the PA system.
- Please adhere to any instructions given over the PA system.
- As a DOE laboratory, we must maintain strict access control to the buildings. Therefore, please stay in this building unless you are escorted by an OLCF staff member.
Miscellaneous Announcements

- If you are interested in meeting with someone on the OLCF staff or elsewhere in the lab and need our help in arranging the meeting, please let us know.

- We have reserved several rooms within this building for additional meeting space. Please see Sherry Ray if you would like to reserve a meeting room while you are here.

- If you are a presenter and have not given us a copy of your slides, please see Ashley Barker or Sherry Ray at the next break so that we can get your presentation loaded on the system as soon as possible.

- We are broadcasting this meeting over BlueJeans for those users that could not join us in person.

- Restrooms and vending machines are located down the hall on the right-hand side.

- There is also a cafeteria located downstairs that is open for both breakfast and lunch.
2018 OLCF User Meeting Survey

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).
Origin of Leadership Computing Facility

Department of Energy High-End Computing Revitalization Act of 2004 (Public Law 108-423):

The Secretary of Energy, acting through the Office of Science, shall

- Establish and operate Leadership Systems Facilities.
- Provide access [to Leadership Systems Facilities] on a competitive, merit-reviewed basis to researchers in U.S. industry, institutions of higher education, national laboratories and other Federal agencies.
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.
OLCF Users’ Publication Yield at All-Time High

Data Snapshot: May 13, 2018
OLCF Users’ Publications Increase in High-Impact Journals

Data Snapshot: May 13, 2018
## Setting Records

<table>
<thead>
<tr>
<th>Measurement</th>
<th>2017 target</th>
<th>2017 actual</th>
<th>2018 YTD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scheduled availability</td>
<td>95%</td>
<td>99.39%</td>
<td>99.54%</td>
</tr>
<tr>
<td>Overall availability</td>
<td>90%</td>
<td><strong>98.09%</strong></td>
<td>99.14%</td>
</tr>
<tr>
<td>Overall User Support Rating</td>
<td>3.5/5.0</td>
<td>4.6</td>
<td>N/A</td>
</tr>
<tr>
<td>User Problem Resolution Time</td>
<td>80% in 3 hrs</td>
<td><strong>93%</strong></td>
<td>97%</td>
</tr>
<tr>
<td>Total usage</td>
<td>NAM</td>
<td><strong>91%</strong></td>
<td>91%</td>
</tr>
<tr>
<td>Core-hours used</td>
<td>NAM</td>
<td>4,389,163,123</td>
<td>1,597,338,620</td>
</tr>
<tr>
<td>Core-hours available</td>
<td>NAM</td>
<td>4,817,215,104</td>
<td>1,746,954,240</td>
</tr>
<tr>
<td>INCITE Capability</td>
<td>NAM</td>
<td>68.22%</td>
<td>46.12%</td>
</tr>
<tr>
<td>Capability - All projects</td>
<td>35%</td>
<td><strong>59.81%</strong></td>
<td>47.56%</td>
</tr>
</tbody>
</table>
What about the Titan component failures?

- 2016 – peak weekly failure rate
- 2017 – completed 11,000 GPU SXM replacements
- 2018 – numbers to date reflect policy enhancements that were enacted in late 2017
What’s next for Titan?

- CUDA 9.2 upgrade to Titan coming soon
  - Currently in testing and evaluation at the OLCF
- Scheduled end-of-life for September 2019 marking 7-years in production
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.

Coming in 2018: Summit will replace Titan as the OLCF’s leadership supercomputer
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™, 1 NVIDIA Kepler™</td>
<td>2 IBM POWER9™, 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>
Installation Nearing Completion

- Hardware installation completed in March
- Continuing to stabilize nodes, disks, and network
- In December, accepted 1,080 of 4,608 nodes to port codes
- OLCF is working with IBM, NVIDIA, Red Hat, and Mellanox to stabilize and debug system software
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.
Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Program for 2019

• Access to the most capable, most productive, fastest open science supercomputers in the nation
• Call for proposals submission window:
  – Apr 16 – Jun 22, 2018
• Applicable to a broad array of science, engineering, and computer science domains
• Proposals must be:
  ° High-impact, computationally and/or data intensive campaigns
  ° Must take advantage of unique HPC architectures
  ° Research that cannot be performed anywhere else.
• INCITE Webinar will be held June 7th
• For more information visit http://www.doeleadershipcomputing.org/
How can you get access to Summit to prepare for INCITE and ALCC competitions?

- CAAR and Early Science Program (ESP) Letter of Intent (LOI) calls are closed;
  - 13 CAAR teams; 60+ ESP-LOI Teams have access to Summit Phase I
  - ESP Proposals due by 1 June 2018,
  - See T. Straatsma’s presentation Wednesday Morning.

- INCITE CFP is open now, closes 22 June 2018.
  - Preparatory access via Titan, Summitdev, and ESP-LOI process on Summit

- DOE’s ALCC program call is expected to open in Fall 2018, expected to close February 2019. For ALCC preparation access:
  - 2018: via Titan, Summitdev, and ESP-LOI process on Summit; Potential to access additional IBM AC922 cluster hardware for application development;
2018 Training Events: Preparing for Summit

• Workshops, webinars, screencasts
• GPU Hackathons
• Mini-GPU-Hackathons

Prepared and presented by OLCF staff, vendors, and partner organizations.
| Jan     | Feb    | Mar            | Apr   | May    | Jun     | Jul     | Aug     | Sep     | Oct     | Nov    | Dec     | Jan     | Feb     |
|---------|--------|----------------|-------|--------|---------|---------|---------|---------|---------|--------|---------|---------|---------|--------|
|                               | Misc. Event Dates |                             |                             |                             |                             |                             |                             |

**Monthly OLCF User Calls**

- Intro to HPC Workshop (6/26 – 6/28)
- Workshop: Targeting Multi-GPU Nodes (TBD)

**Screencasts**

- Hello_jsrun Tool
- Transferring Data between Atlas & AlpineTDS

**GPU Hackathons**

- NCSA (9/10 – 9/14)
- CSCS (10/1 – 10/5)

**Misc. Event Dates**

- Summit Workshop (Jan/Feb)
- ALCC Call closes on 2/1
- INCITE Call closes on 6/22
- INCITE proposal webinars (5/2 and 6/7)
- OLCF User Calls
  - Mar: Profiling with forge (3/28)
  - Apr: CUDA9.2 (4/25)
  - Jun+: TBD
  - OLCF User Meetings
    - Summit Workshop (Jan/Feb)
    - GTC18
    - SC18

**Workshops**

- Summit Workshop (3/5 – 3/9)
- Summit Workshop (10/1 – 10/5)
- Summit Workshop (Jan/Feb)

**Other Information**

- INCITE proposal webinars (5/2 and 6/7)
- OLCF User Calls
  - Mar: Profiling with forge (3/28)
  - Apr: CUDA9.2 (4/25)
  - Jun+: TBD
- Hello_jsrun Tool
- Transferring Data between Atlas & AlpineTDS
- Summit Workshop (Jan/Feb)
Summit will be the world’s smartest supercomputer for open science

But what makes a supercomputer smart?

Summit provides unprecedented opportunities for the integration of artificial intelligence (AI) and scientific discovery. Here’s why:

- **GPU Brawn:** Summit links more than 27,000 deep-learning optimized NVIDIA GPUs with the potential to deliver exascale-level performance (a billion-billion calculations per second) for AI applications.

- **High-speed Data Movement:** NVLink high-bandwidth technology built into all of Summit’s processors supplies the next-generation “information superhighways” needed to train deep learning algorithms for challenging science problems quickly.

- **Memory Where it Matters:** Summit’s sizable local memory gives AI researchers a convenient launching point for data-intensive tasks, an asset that allows for faster AI training and greater algorithmic accuracy.
Science challenges for a smart supercomputer:

Identifying Next-generation Materials
By training AI algorithms to predict material properties from experimental data, longstanding questions about material behavior at atomic scales could be answered for better batteries, more resilient building materials, and more efficient semiconductors.

Predicting Fusion Energy
Predictive AI software is already helping scientists anticipate disruptions to the volatile plasmas inside experimental reactors. Summit’s arrival allows researchers to take this work to the next level and further integrate AI with fusion technology.

Deciphering High-energy Physics Data
With AI supercomputing, physicists can lean on machines to identify important pieces of information—data that’s too massive for any single human to handle and that could change our understanding of the universe.

Combating Cancer
Through the development of scalable deep neural networks, scientists at the US Department of Energy and the National Cancer Institute are making strides in improving cancer diagnosis and treatment.
# Emerging Science Activities: Selected Machine Learning Projects on Titan: 2016-2017

<table>
<thead>
<tr>
<th>Program</th>
<th>PI</th>
<th>PI Employer</th>
<th>Project Name</th>
<th>Allocation (Titan core-hrs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ALCC</td>
<td>Robert Patton</td>
<td>ORNL</td>
<td>Discovering Optimal Deep Learning and Neuromorphic Network Structures using Evolutionary Approaches on High Performance Computers</td>
<td>75,000,000</td>
</tr>
<tr>
<td>ALCC</td>
<td>Gabriel Perdue</td>
<td>FNAL</td>
<td>Large scale deep neural network optimization for neutrino physics</td>
<td>58,000,000</td>
</tr>
<tr>
<td>ALCC</td>
<td>Gregory Laskowski</td>
<td>GE</td>
<td>High-Fidelity Simulations of Gas Turbine Stages for Model Development using Machine Learning</td>
<td>30,000,000</td>
</tr>
<tr>
<td>ALCC</td>
<td>Efthimions Kaxiras</td>
<td>Harvard U.</td>
<td>High-Throughput Screening and Machine Learning for Predicting Catalyst Structure and Designing Effective Catalysts</td>
<td>17,500,000</td>
</tr>
<tr>
<td>ALCC</td>
<td>Georgia Tourassi</td>
<td>ORNL</td>
<td>CANDLE Treatment Strategy Challenge for Deep Learning Enabled Cancer Surveillance</td>
<td>10,000,000</td>
</tr>
<tr>
<td>DD</td>
<td>Abhinav Vishnu</td>
<td>PNNL</td>
<td>Machine Learning on Extreme Scale GPU systems</td>
<td>3,500,000</td>
</tr>
<tr>
<td>DD</td>
<td>J. Travis Johnston</td>
<td>ORNL</td>
<td>Surrogate Based Modeling for Deep Learning Hyper-parameter Optimization</td>
<td>3,500,000</td>
</tr>
<tr>
<td>DD</td>
<td>Robert Patton</td>
<td>ORNL</td>
<td>Scalable Deep Learning Systems for Exascale Data Analysis</td>
<td>6,500,000</td>
</tr>
<tr>
<td>DD</td>
<td>William M. Tang</td>
<td>PPPL</td>
<td>Big Data Machine Learning for Fusion Energy Applications</td>
<td>3,000,000</td>
</tr>
<tr>
<td>DD</td>
<td>Catherine Schuman</td>
<td>ORNL</td>
<td>Scalable Neuromorphic Simulators: High and Low Level</td>
<td>5,000,000</td>
</tr>
<tr>
<td>DD</td>
<td>Boram Yoon</td>
<td>LANL</td>
<td>Artificial Intelligence for Collider Physics</td>
<td>2,000,000</td>
</tr>
<tr>
<td>DD</td>
<td>Jean-Roch Vlimant</td>
<td>Caltech</td>
<td>HEP DeepLearning</td>
<td>2,000,000</td>
</tr>
<tr>
<td>DD</td>
<td>Arvind Ramanathan</td>
<td>ORNL</td>
<td>ECP Cancer Distributed Learning Environment</td>
<td>1,500,000</td>
</tr>
<tr>
<td>DD</td>
<td>John Cavazos</td>
<td>U. Delaware</td>
<td>Large-Scale Distributed and Deep Learning of Structured Graph Data for Real-Time Program Analysis</td>
<td>1,000,000</td>
</tr>
<tr>
<td>DD</td>
<td>Abhinav Vishnu</td>
<td>PNNL</td>
<td>Machine Learning on Extreme Scale GPU systems</td>
<td>1,000,000</td>
</tr>
<tr>
<td>DD</td>
<td>Gabriel Perdue</td>
<td>FNAL</td>
<td>MACHINE Learning for MINERvA</td>
<td>1,000,000</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td></td>
<td></td>
<td></td>
<td><strong>220,500,000</strong></td>
</tr>
</tbody>
</table>
OLCF Accelerating ML/AI Deployment for Science

1. Establishing early science and significant applications
   - Summit/Dev Early Science Applications (e.g., CANDLE)
   - INCITE projects (e.g., Co-evolutionary Networks: From Genome to 3D Proteome, Jacobson, et al.)
   - Directors Discretion (e.g., Fusion RNN, MiNerva)

2. Creating leadership class analytics capabilities
   - Leadership analytics (e.g., Frameworks: pbdR, TensorFlow + Horovod)
   - Large-scale targeted algorithms (e.g., non-negative matrix factorization)

3. Enabling infrastructure for analytics/AI
   - Workflows to include data from observations for analysis within OLCF
   - Analytics enabling technologies (e.g., container deployments for rapidly changing DL/ML frameworks, analytic notebooks, etc.)
Enabling Leadership Science: Data, Simulation, and Analytics at Scale

- Cross-Facility Workflows
- Platform as a service (e.g., OpenShift)
- Container Deployments
- Machine Learning/Deep Learning at Scale

Workflows:
- Staging and Cross-System and Cross-Facility
- Well-known runtime and programming language extensions, ...

Capability Compute at OLCF:
- Simulation & Compute/Data Workflows at Scale
- ADIOS
- OpenShift, OpenStack
- Singularity

Data On-Ramps: Observational Data
- Scalable Computing
- CADES, ...
- Cloud, SHPC, DGX, Urika, Applications
- Globus
- PANDA, Fireworks, Pegasus, Swift, ...

Data Life-Cycle:
- Dissemination, Sharing, Analytics Products
- Constellation
- EDEN, Visit, Paraview, SIGHT
- CrossBOW
- Support: PDACS, Galaxy, Zeppelin, ...

Analytics:
- Analysis at Scale
- Visual Analytics
- pbdR
- Spark on Demand
- TensorFlow, pyTorch, Keras, Caffe, MxNet

Artifacts and Insights

- Support: PDACS, Galaxy, Zeppelin, ...
- OpenShift, OpenStack
- Singularity
In April 2018, DOE Secretary Rick Perry announced an open, competitive solicitation for exascale computers to be delivered in 2021 and 2022 known as the CORAL-2 Request For Proposals

http://procurement.ornl.gov/rfp/CORAL2/

• The designs for these computers will target a 50x increase in scientific application performance over current DOE leadership computers.

• CORAL will award up to 3 computer systems
  – beginning with a 2021 installation at Oak Ridge National Laboratory, with the requirement that the system must be diverse from the ALCF 2021 system
  – followed by a 2022 installation at Lawrence Livermore National Laboratory
  – with the potential for a 3rd system at Argonne National Laboratory

• Responses to this solicitation are due on May 24, 2018
The Exascale Computing Project has emphasized that Exascale is a measure of application performance, and this RFP reflects that, asking for nominally 50× improvement over Sequoia and Titan.

-- Design Reviewer
2021 delivery planned with >1000 PF performance (50–100× the scientific productivity of current Titan system)

Frontier NRE: hardware and software engineering
- Prepare power, cooling, and space
- Installation
- Prepare scientific software applications
- Frontier available

Summit available: 200 PF production system

Titan available: 27 PF

The OLCF User Group (OUG)
https://www.olcf.ornl.gov/about-olcf/oug/

• “The purpose of OUG is to provide advice and feedback to the OLCF on the current and future state of OLCF operations and services.”

• The OUG Executive Board represents OUG to the OLCF and serves as advocates for the OLCF user community.

• Six users are running for three open positions on the board this year: https://tinyurl.com/OUGElection2018

• Vote until Thursday, May 17th 9AM EDT: https://tinyurl.com/OUGVote2018

• Results will be announced at the conclusion of the User Meeting
2018 OLCF User Meeting Survey