Beyond the CPU: Is Accelerated Computing for Everyone?

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Director of Science
National Center for Computational Sciences
Oak Ridge National Laboratory

VP OpenACC Consortium

SC19, Denver

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The U.S. Department of Energy’s Oak Ridge National Laboratory is the largest US Department of Energy (DOE) open science laboratory.
Mission: Deploy and operate the computational resources required to tackle global challenges

- Provide world-leading computational and data resources and specialized services for the most computationally intensive problems
- Provide stable hardware/software path of increasing scale to maximize productive applications development
- Operate world-class user programs accessible to industry, universities, national laboratories and federal agencies, with access is based on the merit of the proposed work.
- With our partners, deliver transforming discoveries and engineering breakthroughs across a breadth of applications.
Origin of Leadership Computing Facility Program

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.”
Who's Been Working With Us?
Industrial Use of OLCF by Fiscal Year

- **New Projects Launched in Fiscal Year**
- **Projects Carried over from Previous Year(s)**

<table>
<thead>
<tr>
<th>Fiscal Year</th>
<th>New Projects</th>
<th>Carried over</th>
</tr>
</thead>
<tbody>
<tr>
<td>2006</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>2007</td>
<td>5</td>
<td>5</td>
</tr>
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<td>2008</td>
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<tr>
<td>2009</td>
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<td>3</td>
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<td>2010</td>
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<td>12</td>
</tr>
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<td>2011</td>
<td>9</td>
<td>14</td>
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<td>2012</td>
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<td>2013</td>
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<td>2014</td>
<td>28</td>
<td>21</td>
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<tr>
<td>2015</td>
<td>39</td>
<td>36</td>
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<tr>
<td>2016</td>
<td>42</td>
<td>20</td>
</tr>
<tr>
<td>2017</td>
<td>42</td>
<td>17</td>
</tr>
<tr>
<td>2018</td>
<td>43</td>
<td>23</td>
</tr>
<tr>
<td>2019</td>
<td>40</td>
<td>21</td>
</tr>
</tbody>
</table>

- **Year Notes**
  - New Projects Launched in Fiscal Year
  - Projects Carried over from Previous Year(s)
Science Impact – Publications Growth

• In 2018, OLCF staff and users have published 472 peer-reviewed articles. This is an OLCF maximum yield.

• Annual publications (User + Staff) at all-time high for the past three successive years (CY16, CY17, CY18.
No more free lunch: Moore’s Law continues, Denard Scaling is over

42 Years of Microprocessor Trend Data

Transistors (thousands)

Single-Thread Performance (SpecINT x 10^3)

Frequency (MHz)

Typical Power (Watts)

Number of Logical Cores

Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten

New plot and data collected for 2010-2017 by K. Rupp

https://www.karlrupp.net/2018/02/42-years-of-microprocessor-trend-data/
ORNL has systematically delivered a series of leadership-class systems
On scope • On budget • Within schedule

OLCF-1

2004 Cray X1E Phoenix
18.5 TF

2005 Cray XT3 Jaguar
25 TF

2006 Cray XT3 Jaguar
54 TF

2007 Cray XT4 Jaguar
62 TF

2008 Cray XT4 Jaguar
2008
263 TF

2009 Cray XT5 Jaguar
1 PF

2009 Cray XT5 Jaguar
2.5 PF

2012 Cray XK7 Titan
27 PF

1000-fold improvement in 8 years

2007 CUDA Initial Release

OLCF-2

OLCF-3
GPUs provided a path forward using Hierarchical Parallelism

- Expose more parallelism through code refactoring and source code directives
  - Doubles CPU performance of many codes

- Use right type of processor for each task

- Data locality: Keep data near processing
  - GPU has high bandwidth to local memory for rapid access
  - GPU has large internal cache

- Manage data movement between CPU and GPU memories
Titan’s Node Architecture

- DRAM: 32 GB
- GDDR: 6 GB
- GPU: 1.4 TF
- PCIe Gen2: 55 GB/s
- GDDR/DRAM Bus (aggregate B/W): 250 GB/s
- x86: 5 GB/s
We are building on this record of success to enable exascale in 2021

➢ From Titan to Summit, 8-fold improvement
➢ From Titan to Frontier, 50-fold improvement
➢ From Jaguar to Frontier, 500-fold improvement

Titan was decommissioned August 2019.
ORNL Debuted Summit Supercomputer: June 8, 2018

• ORNL launched the Summit IBM AC922, the world’s most powerful and smartest scientific supercomputer, on June 8. Energy Secretary Rick Perry, Tennessee Governor Bill Haslam, and the CEOs of IBM and NVIDIA were present to celebrate the announcement.

• Attending the June 8 launch were (left to right) Tennessee Governor Bill Haslam, US Secretary of Energy Rick Perry, IBM CEO Ginni Rometty, ORNL lab director Thomas Zacharia, and NVIDIA CEO Jensen Huang.

ORNL has launched its newest supercomputer: the IBM AC922 Summit, located at the OLCF.
Summit is latest DOE #1 system on Top500

143.5 PF HPL
Shows math performance

2.9 PF HPCG
Shows fast data movement

#1 on the IO-500
Shows file system performance

14.7 GF/W
Shows energy efficiency
Summit Node Schematic

- Coherent memory across entire node
- NVLink v2 fully interconnects three GPUs and one CPU on each side of node
- PCIe Gen 4 connects NVM and NIC
- Single shared NIC with dual EDR ports
Experimental and simulated data set volumes are growing exponentially. Examples: High luminosity LHC, light sources, climate, cosmology data sets ~ 100s of PBs.

Methods and workflows of data analytics are different than those in traditional HPC. Machine learning is revolutionizing field. Established analysis programs must be accommodated.

DOE exascale ecosystem requirements reviews: http://exascaleage.org/
## OLCF Training Program: Tom Papatheodore, leader

<table>
<thead>
<tr>
<th>Category</th>
<th>Description</th>
<th>Resources</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Introduction to HPC</strong></td>
<td>intro topics + traditional classroom-style</td>
<td><a href="https://www.olcf.ornl.gov/calendar/introduction-to-hpc/">https://www.olcf.ornl.gov/calendar/introduction-to-hpc/</a></td>
</tr>
<tr>
<td><strong>App Teams</strong></td>
<td>hands-on + application readiness</td>
<td><a href="https://www.olcf.ornl.gov/for-users/training/gpu-hackathons/">https://www.olcf.ornl.gov/for-users/training/gpu-hackathons/</a></td>
</tr>
<tr>
<td><strong>Special Topics &amp; Tutorials</strong></td>
<td>current topics + scientific domains</td>
<td><a href="https://github.com/olcf-tutorials">https://github.com/olcf-tutorials</a></td>
</tr>
</tbody>
</table>

[https://www.olcf.ornl.gov/for-users/training/training-archive/](https://www.olcf.ornl.gov/for-users/training/training-archive/)
GPU Hackathons Impact

### Number of Codes Accelerated at Hackathons (cumulative)

<table>
<thead>
<tr>
<th>Year</th>
<th>2015</th>
<th>2016</th>
<th>2017</th>
<th>2018</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>21</td>
<td>46</td>
<td>93</td>
<td>191</td>
</tr>
</tbody>
</table>

### Hackathon Hosting Institutions

- Oak Ridge National Laboratory
- CSCS
- Pawsey Supercomputing Centre
- HZDR
- MIT
- JGI
- Helmholtz Zentrum Dresden Rossendorf
- University of Delaware
- Princeton University
- Tsinghua University
- CDAC
- Jülich Research Centre
- Brookhaven National Laboratory
- University of Colorado Boulder
- National Supercomputing Center in Shenzhen
- Shenzhen Cloud Computing Center

### Number of Hackathons

<table>
<thead>
<tr>
<th>Year</th>
<th>2015</th>
<th>2016</th>
<th>2017</th>
<th>2018</th>
<th>2019</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>8</td>
<td>16</td>
</tr>
</tbody>
</table>

~25 hackathons in 2020

### So far in 2019...

- 60+ application teams
- 400+ attendees
- 80+ institutions

https://www.gpuhackathons.org/

papatheodore@ornl.gov
TRAINING AND EDUCATION
ORNL Leader: papatheodore@ornl.gov
OpenACC Leader: jlevites@nvidia.com

GPU Hackathons and Bootcamps

GPU Bootcamps

- 1 or 2-day event
- Labs and a mini-app challenge
- 50 people with 2-3 mentors
- Prepare for future hackathons and start collaborations

Hackathons

- 5-day event
- Users bring their own codes or data
- Up to 10 teams with 3+ people per team
- 2 mentors per team

Number of Hackathons

<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Count</td>
<td>1</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>8</td>
<td>15</td>
<td>20</td>
</tr>
</tbody>
</table>

1270 participants trained

23 Bootcamps in 2019

40 Bootcamps in 2020

Codes Accelerated at Hackathons (cumulative)

<table>
<thead>
<tr>
<th>Year</th>
<th>2015</th>
<th>2016</th>
<th>2017</th>
<th>2018</th>
<th>2019</th>
</tr>
</thead>
<tbody>
<tr>
<td>Codes</td>
<td>21</td>
<td>46</td>
<td>93</td>
<td>191</td>
<td>300</td>
</tr>
</tbody>
</table>

www.gpuhackathons.org
## SELECTED HACKATHONS HIGHLIGHTS

<table>
<thead>
<tr>
<th>Code</th>
<th>Domain</th>
<th>Result in 5 days</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHARMM</td>
<td>MD</td>
<td>7.5x on a kernel</td>
</tr>
<tr>
<td>LAVA(NASA)</td>
<td>CFD</td>
<td>10x on a mini-app</td>
</tr>
<tr>
<td>HiFUN</td>
<td>CFD</td>
<td>3.2x on a full app, 100x on a kernel</td>
</tr>
<tr>
<td>Yambo</td>
<td>QC</td>
<td>6x on a full app</td>
</tr>
<tr>
<td>CASTRO</td>
<td>Astro</td>
<td>14x on mini-app</td>
</tr>
<tr>
<td>Garnet</td>
<td>Earth Sciences</td>
<td>40x on mini-app</td>
</tr>
<tr>
<td>CGYRO</td>
<td>Physics</td>
<td>10x on a mini-app</td>
</tr>
<tr>
<td>CASTEP</td>
<td>QC</td>
<td>2.7x and 11x on 2 parts</td>
</tr>
<tr>
<td>SPECFEM-X</td>
<td>Geophysics</td>
<td>205x vs single CPU core</td>
</tr>
<tr>
<td>GTS</td>
<td>Fusion</td>
<td>25x for the kernel and 3x for the overall app</td>
</tr>
<tr>
<td>Quantum Espresso</td>
<td>QC</td>
<td>6x on a part of the code</td>
</tr>
<tr>
<td>DFT-FE</td>
<td>Quantum Mechanics</td>
<td>40x on kernels</td>
</tr>
</tbody>
</table>

I’m a firm believer in **collaborative science**, and it was wonderful to see several of my graduate students and postdocs deeply engaged. The team made tremendous progress during the week, and that momentum has carried the project forward ever since. In four days they managed to obtain a two-orders-of-magnitude increase in performance, and since then they’ve made further optimizations that gained them another order of magnitude. This speedup has opened up an entirely new class of problems in quasistatic global geophysics. From my perspective, this was a very successful event!

*Jeroen Tromp, Blair Professor of Geology and Professor of Applied & Computational Mathematics at Princeton University*
OPENACC ORGANIZATION MISSION

The OpenACC Organization is dedicated to helping the research and developer community advance science by expanding their accelerated and parallel computing skills. We have 3 areas of focus: participating in computing ecosystem development, providing training and education on programming models, resources and tools, and developing the OpenACC specification.
PILLARS OF OPENACC ORGANIZATION

ECOSYSTEM DEVELOPMENT

Work with Language Standards committees
- Apply collective lessons learned
- Bridge gaps in base languages
- Develop roadmap for interoperability

Strive for performant interoperability

TRAINING & EDUCATION

Hackathons/Bootcamps
- Focus on accelerated computing

Training Materials:
- Courses
- Containers
- Workshops

Programs for educators, students, mentors

OPENACC SPECIFICATION

Develop OpenACC Specification by introducing new features and functionality
ECOSYSTEM DEVELOPMENT

APPLICATIONS

BASE AND DOMAIN SPECIFIC LANGUAGES

HIGH LEVEL MODELS & LIBRARIES

DIRECTIVES

PLATFORM-SPECIFIC ENVIRONMENTS

Enabling Performant Interoperability
OPENACC DIRECTIVES

a directive-based parallel programming model designed for usability, performance and portability

3 OF TOP 5 HPC

18% OF INCITE AT SUMMIT

PLATFORMS SUPPORTED

OPENACC APPS

OPENACC SLACK MEMBERS

>200K DOWNLOADS

NVIDIA GPU
X86 CPU
POWER CPU
Sunway
ARM CPU
AMD GPU
Accelerator Programming Models on Summit - 2019 INCITE

Accelerator Programming Model: Runtime Weighted

- Summit Accelerator Programming Models, Runtime Weighted
  - (1) 75.1% CUDA (includes RAJA, KOKKOS)
  - (2) 17.5% OPENACC
  - (3) 3.9% CUDA Fortran
  - (4) 3.6% OPENMP

➢ OpenACC programming model is critically important for Summit’s user programs

Programming model weighted by consumed-hours for INCITE up to September 2019

Source: XALT / Reuben Budiardja, NCCS

NOTES:
- Programming model weighted by consumed-hours.
- Using XALT, RAJA & KOKKOS use show up as CUDA
Base languages in 2019 INCITE on Summit

Languages: Runtime Weighted

- C: 10.1%
- Fortran: 38.0%
- C++: 51.9%

Modern FORTRAN required as a “first-class” citizen in our user programs.

Based on usage up to September 2019, results will continue to change.
Accelerator Programming Models for **Fortran Codes** on Summit - 2019 INCITE

**Summit Accelerator Programming Models, Fortran Code - Runtime Weighted**

1. 43.1% OPENACC
2. 38.5% CUDA (includes RAJA, KOKKOS)
3. 9.6% CUDA Fortran
4. 8.8% OPENMP

➢ OpenACC programming model is critically important for Summit’s user programs

NOTES:
- Programming model weighted by consumed-hours.
- Using XALT, RAJA & KOKKOS use show up as CUDA

Programming model weighted by consumed-hours for INCITE up to September 2019

Source: XALT / Reuben Budiardja, NCCS
Frontier Overview

Partnership between ORNL, Cray, and AMD
The Frontier system will be delivered in 2021
Peak Performance greater than 1.5 EF
Composed of more than 100 Cray Shasta cabinets
  - Connected by Slingshot™ interconnect with adaptive routing, congestion control, and quality of service

Node Architecture:
  - An AMD EPYC™ processor and four Radeon Instinct™ GPU accelerators purpose-built for exascale computing
  - Fully connected with high speed AMD Infinity Fabric links
  - Coherent memory across the node
  - 100 GB/s injection bandwidth
  - Near-node NVM storage
## Migration Path from Summit to Frontier

<table>
<thead>
<tr>
<th>Summit</th>
<th>Frontier</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>CUDA C/C++</td>
<td>HIP C/C++</td>
<td>HIP provides tools to help port existing CUDA codes to the HIP layer.</td>
</tr>
<tr>
<td>OpenACC</td>
<td>OpenMP (offload)</td>
<td>OpenACC codes can be migrated to OpenMP (offload) for Frontier. <strong>Direct support for OpenACC on Frontier is still under discussion.</strong></td>
</tr>
<tr>
<td>OpenMP (offload)</td>
<td>OpenMP (offload)</td>
<td>Virtually the same on Summit and Frontier</td>
</tr>
<tr>
<td>Fortran w/CUDA C/C++</td>
<td>Fortran w/HIP C/C++</td>
<td>As with CUDA, this will require interfaces to the C/C++ API calls</td>
</tr>
<tr>
<td>CUDA FORTRAN</td>
<td>FORTRAN w/HIP C/C++</td>
<td>As with CUDA, this will require interfaces to the C/C++ API calls</td>
</tr>
</tbody>
</table>

[https://www.olcf.ornl.gov/frontier/](https://www.olcf.ornl.gov/frontier/)
GCC: Most Frequently Used Compiler Family

**Compiler Count By Family CY-2019**

January - September, Total Count: ~2.7M

- Clang & Clang++: 1.1%
- IBM XL: 22.7%
- PGI: 7.5%
- GCC: 68.7%
RFP for Work on GCC Compiler Suite

Ensure that OpenACC is performant on Frontier through GCC

• OLCF will enable up-to-date implementations of OpenACC and OpenMP standards within the GCC compiler suite up to the latest versions of the standards.

• A “Request for Proposals” was opened Aug. 29, 2019.
  – Support the GPUs of immediate interest to OLCF (NVIDIA & AMD) so that OpenACC becomes fully capable for OLCF users on Summit, Frontier, and other platforms.

• The expectation is that this work will be completed as quickly as reasonably possible, but prior to April 2022, in anticipation of the upcoming delivery of the new Frontier system.
Summary & Conclusions

- Titan is gone; Summit is here; Frontier is coming for users in 2022.
- Training and education is a critical component of enabling accelerated computing deliver on its opportunities.
- OpenACC directives approach is very important for OLCF user programs.
- Community-focused GPU Hackathons are having a big impact.
- OLCF is increasing investments in GCC to make OpenACC and OpenMP performant on Summit and Frontier.
Acknowledgment

XALT data is supported by a team effort behind the scene:

- Bill Renaud diligently keeps XALT operational data current
- Jason Kincl set up services on Kubernetes cluster / Openshift for analysis
- Ryan Prout helped set up XALT data flows through Apache Kafka
Questions & Discussion

Jack Wells, wellsjc@ornl.gov