Data Science at OLCF

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OLCF Data/Learning Strategy & Tactics

1. Engage with applications
   - Summit Early Science Applications (e.g., CANDLE)
   - INCITE projects (e.g., Co-evolutionary Networks: From Genome to 3D Proteome, Jacobson, et al.)
   - Directors Discretionary projects (e.g., Fusion RNN, MiNerva)

2. Create leadership-class analytics capabilities
   - Leadership analytics (e.g., Frameworks: pbdR, TensorFlow + Horovod)
   - Algorithms requiring scale (e.g., non-negative matrix factorization)

3. Enable infrastructure for analytics/AI and data-intensive facilities
   - Workflows to include data from observations for analysis within OLCF
   - Analytics enabling technologies (e.g., container deployments for rapidly changing DL/ML frameworks, analytics notebooks, etc.)
Applications Supported through DD/ALCC: 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>
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<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>
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<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>
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<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>
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<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>
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<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>
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<tr>
<td>DD</td>
<td>J. Travis Johnston</td>
<td>ORNL</td>
<td>Surrogate Based Modeling for Deep Learning Hyper-parameter Optimization</td>
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<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>
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<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>
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<td>DD</td>
<td>Catherine Schuman</td>
<td>ORNL</td>
<td>Scalable Neuromorphic Simulators: High and Low Level</td>
<td>5,000,000</td>
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<tr>
<td>DD</td>
<td>Boram Yoon</td>
<td>LANL</td>
<td>Artificial Intelligence for Collider Physics</td>
<td>2,000,000</td>
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<tr>
<td>DD</td>
<td>Jean-Roch Vlimant</td>
<td>Caltech</td>
<td>HEP DeepLearning</td>
<td>2,000,000</td>
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<tr>
<td>DD</td>
<td>Arvind Ramanathan</td>
<td>ORNL</td>
<td>ECP Cancer Distributed Learning Environment</td>
<td>1,500,000</td>
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<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>
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<tr>
<td>DD</td>
<td>Abhinav Vishnu</td>
<td>PNNL</td>
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<td>1,000,000</td>
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<tr>
<td>DD</td>
<td>Gabriel Perdue</td>
<td>FNAL</td>
<td>MACHINE Learning for MINERvA</td>
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<td><strong>TOTAL</strong></td>
<td><strong>220,500,000</strong></td>
</tr>
</tbody>
</table>

- Highlighted rows are Algorithm and Infrastructure Examples; Rest are Primarily Science Applications

Acknowledgement: J. Wells, SC 2017
Gordon Bell Prizes in 2018: Peak Performance on Summit

Attesting the Opioid Epidemic: Determining the Epistatic and Pleiotropic Genetic Architectures for Chronic Pain and Opioid Addiction
Wayne Joubert, Deborah Weighill, David Kainer, Sharlee Climer, Amy Justice, Kjiersten Fagnan, Daniel Jacobson

Exascale Deep Learning for Climate Analytics
Thorsten Kurth, Sean Treichler, Joshua Romero, Mayur Mudigonda, Nathan Luehr, Everett Phillips, Ankur Mahesh, Michael Matheson, Jack Deslippe, Massimiliano Fatica, Prabhat, Michael Houston,
Methods: Leadership Data Analytics Capabilities

- Significantly improved throughput compared to, e.g., Apache Spark
  - “PCA of a 134 GB matrix: ‘hours on . . . Apache Spark, . . . less than a minute using R.’”
  - June 2016, HPCWire
Scaling Deep Learning for Science with ORNL’s MENNDL

**ORNL-designed algorithm leverages Titan to create high-performing neural networks**

An image generated from neutrino scattering data captured by the MINERvA detector at Fermi National Accelerator Laboratory. Researchers are using MENNDL and the Titan supercomputer to generate deep neural networks that can classify high-energy physics data and improve the efficiencies of measurements.

## Key Data Science and Learning Methods

<table>
<thead>
<tr>
<th>CORAL 2 Benchmark Suite</th>
<th>Components</th>
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<tbody>
<tr>
<td>Big Data Analytic Suite (BDAS)</td>
<td>PCA, K-Means, and SVM (based on pbdR)</td>
</tr>
<tr>
<td>Deep Learning Suite (DLS)</td>
<td>CANDLE, CNN, RNN, and ResNet-50 (distributed memory)</td>
</tr>
</tbody>
</table>

Deep Learning Codes (CNN; ResNet50; ..) excel here with NVM and GPUs enabling tensor operations.

PCA, K-Means, etc. excel on “traditional HW” part of the node due to the node’s memory, CPU, and on-chip bandwidth.

Big Data Analytic Suite

Speedup Over Titan Baseline for CORAL-2
Big Data Benchmarks (based on pbdR)

Weak Scaling of Data Benchmarks on Titan

Strong Scaling of Data Benchmarks on SummitDev

Wall time (seconds) vs. # of nodes

Wall time (seconds) vs. # of nodes
Deep Learning Suite

Speedup Over Titan Baseline for CORAL-2 Deep Learning Benchmarks

- SummitDev
- Summit

CANDLE: x3.5 x5.9
RNN: x4
CNN-googlenet: x6
CNN-vgg: x4 x6
CNN-alexnet: x4 x6
CNN-overfeat: x4 x6

Strong Scaling of ResNet-50 on Summit

Scaling of ResNet-50 based on Keras (Tensorflow backend) and Horovod on ImageNet data

seconds/epoch

actual

ideal

2000
200
20

24 48 96 192 384 # of GPUs
Infrastructure - Cross-Facility Design Pattern

From: Policy Considerations when Federating Facilities for Experimental and Observational Data Analysis, Mallikarjun (Arjun) Shankar, Suhas Somnath, Sadaf Alam, Derek Feichtinger, Leonardo Sala, and Jack Wells, (2018, Submitted Book Chapter)
CADES runs BEAM and Pycroscopy for SNS and CNMS

Towards Data Service Offerings and Easier Data Access Across Facilities

• Categories of Data Services
  – **Type 1** data repository program for “data-only” projects.
  – **Type 2** data services program for user communities.
  – **Type 3** computational and data science end station program.

• “DataFed” prototype to enable federated data access across facilities (currently being tested)

Data Services Program POC: Val Anantharaj; DataFed POC: Dale Stansberry