Big Data Center

Prabhat
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NERSC: the Mission HPC Facility for DOE
Office of Science Research

Largest funder of physical science research in the U.S.

Bio Energy, Environment
Computing
Materials, Chemistry, Geophysics

Particle Physics, Astrophysics
Nuclear Physics
Fusion Energy, Plasma Physics

7,000 users, 700 projects, 700 codes, 48 states, 40 countries, universities & national labs
<table>
<thead>
<tr>
<th>Capabilities</th>
<th>Technologies</th>
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<tbody>
<tr>
<td>Data Transfer + Access</td>
<td>globus online, GridFTP, jupyter, !M, python, django, newt</td>
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<tr>
<td>Workflows</td>
<td>FireWorks, taskfarmer</td>
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<tr>
<td>Data Management</td>
<td>HDF, netCDF, MongoDB, MySQL, PostgreSQL</td>
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<tr>
<td>Data Analytics</td>
<td>python, Spark, TensorFlow, PyTorch, R, julia, Caffe, K</td>
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<td>Data Visualization</td>
<td>VISIT, ParaView</td>
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## Deep Learning Stack

<table>
<thead>
<tr>
<th>Deep Learning Frameworks</th>
<th>Technologies</th>
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<tr>
<td>TensorFlow</td>
<td>Theano, Neon, CNTK, MXNet, …</td>
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<tr>
<td>Caffe</td>
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<td>PyTorch</td>
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<tr>
<th>Multi Node libraries</th>
<th>GRPC</th>
<th>MLSL</th>
<th>Cray Plugin</th>
<th>Horovod</th>
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<th>Single Node libraries</th>
<th>MKL-DNN</th>
<th>CuDNN</th>
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<tr>
<th>Hardware</th>
<th>CPUs (KNL)</th>
<th>GPUs</th>
<th>FPGAs</th>
<th>Accelerators</th>
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Big Data Center

What are Data *capability* applications?
What is the software strategy?
How do we utilize HPC hardware?
Mission:
Solve DOE’s leading data-intensive science problems at scale on Cori

Performance Optimization and Scaling of Production Data Analytics and Management Technologies
Big Data Center Collaboration

intel®

NERSC

CRAY

Berkeley
UNIVERSITY OF CALIFORNIA

UC DAVIS
UNIVERSITY OF CALIFORNIA

[Logos of other institutions]

NYU
Creating a catalog of all visible objects in the Universe
Celeste: 1st Julia application to achieve 1PF

**Scientific Achievement**
- First catalog with parameter and *uncertainty* estimates for 188M objects
- 55 TB SDSS dataset processed in 15 minutes on Cori @ NERSC
- DESI instrument will use catalog for target selection

**Statistics Achievement**
- Bayesian Inference on world’s largest generative model (in science)
- Joint estimation of 8B parameters

**CS Achievement**
- Code written in Julia, optimized for execution on KNL
- Code scaled on 9300 KNL nodes
- Uses BB for staging data
Celeste 2.0: Graphical Model + Deep Learning

- Jeff Regier, Bryan Liu, Jon McAuliffe (UCB); Andy Miller, Ryan Adams (Harvard); David Schlegel (LBL Physics)

- Auto-encoder and RNN for modeling variable number of light sources
- Gravitational Lensing
Determining the Fundamental Constants of Cosmology
Galactos

• **Scientific Achievement**
  – Computed 3-pt correlation for the largest scientific dataset (2B galaxies from Outer Rim) in ~20 minutes
  – Code is ready for LSST: 10B galaxies

• **Methods Achievement**
  – Novel O(N^2) algorithm based on spherical harmonics

• **CS Achievement**
  – Optimized KD-tree for spatial partitioning and querying
  – Single node implementation achieves 39% peak (max: 50%)
  – Code achieves 9.8PF (mixed precision)
CosmoFlow

- Amrita Mathuriya (Intel); Debbie Bard (NERSC); Pete Mendygral (Cray); Siyu He, Shirley Ho (LBL Physics); et al.
- 3D CNN implemented in TensorFlow scaled to 8192 Cori/KNL nodes with Cray DL plugin. 3.5 PF peak performance.
Characterizing Extreme Weather in a Changing Climate
SC’17:: Deep Learning at 15PF

- **Scientific Achievement**
  - Unified architecture for climate pattern classification

- **Methods Achievement**
  - Semi-supervised convolutional architecture
  - Hybrid parameter update strategy

- **CS Achievement**
  - IntelCaffe + MLSL optimized on KNL
  - 2TF peak on single KNL node
  - 15 PF peak on 9300 Cori nodes
Topological Analysis

- Vitaliy Kurlin, Grzegorz Muszynski (U. Liverpool); Karthik Kashinath (NERSC)

- Method is independent of threshold specification
- Classification accuracy for Atmospheric Rivers: 91%
DisCo

- Adam Rupe, Jim Crutchfield (UC Davis); Nalini Kumar (Intel); Karthik Kashinath (NERSC); et al.
- Unsupervised pattern *discovery* technique based on computational mechanics; capable of recovering coherent flow structures
- Implemented in Python
Understanding the Fundamental Constituents of Matter
Graph NNs for Neutrino classification

- Nick Choma, Joan Bruna (NYU); Federico Monti, Michael Bronstein (ICS, U. Svizzera); Spencer Klei, Tomasz Palczewski (LBL Physics); Lisa Gerhardt, Wahid Bhimji (NERSC)
• Frank Wood (UBC); Gunes Baydin (Oxford); Kyle Cranmer (NYU); Lei Shao (Intel); Wahid Bhimji (NERSC); et al.

• Goal: Pattern classification and anomaly detection on HEP data

• Approach: Combine Probabilistic Programming and Deep Learning

• Dynamic, hybrid 3D Conv + LSTM architecture
Data Analytics on Cori

# users

1K cores 10K cores 100K cores 1M cores

SC’17 SC’18 SC’19

R, Spark, Python, PyTorch, TensorFlow, Julia, Caffe

1K cores 10K cores 100K cores 1M cores
Broader Deployment / Availability

• Performance enhancements incorporated into builds of Julia, Caffe, TensorFlow, MKL-DNN, MLSL, Cray DL plugin, ...

• NERSC software builds and documentation has been updated

• Select applications being converted to benchmarks
  – Deep Learning benchmark suite for analytics
  – Celeste I/O benchmark
  – ‘Workflow’ benchmark
Conclusions

• Big Data Center collaboration is enabling capability applications on Cori
  – NERSC: Domain Science drivers in Astronomy, Cosmology, Climate and HEP
  – IPCCs: State-of-the-art research in Deep Learning, Graphical Models, Probabilistic Programming, Topological Methods and Computational Mechanics
  – Intel and Cray: Performance Optimization and Scaling of Production Data Analytics and Management technologies

• We intend to share lessons learnt, code, benchmarks with the broader community

• We welcome collaborations!
Thank You!