Berkeley Lab Computational Research Update

CCS - LBL Collaborative Workshop
April 10, 2014

David L. Brown
Computational Research Division Director
Berkeley Lab at a Glance

- Solve the most pressing and profound scientific problems facing humankind
  - Basic science for a secure energy future
  - Understand living systems to improve the environment and energy supply
  - Understand matter and energy in the universe
- Build and safely operate world-class scientific facilities
- Train the next generation of scientists and engineers

Berkeley Lab’s largest research facilities see more than 25,000 users per year

- Advanced Light Source
- Molecular Foundry
- National Center for Electron Microscopy
- National Energy Research Scientific Computing Center (NERSC)
- 88-Inch Cyclotron
- Joint Genome Institute
- Energy Sciences Network (ESnet)

FY 2011 Total
$734M core, $89M ARRA

3,863 FTE
3,040 Employees
267 Joint faculty
491 Postdoctoral researchers
328 Graduate students
194 Undergraduates
1,612 Visiting scientists and engineers
We are working to enable new experimental science capabilities through advanced math and computing.
CRT Location Supports Collaboration with University of California at Berkeley

- Computer Science
- Electrical Engineering
- Mathematics
- CSE graduate program office
- Berkeley Institute for Data Sciences
- Simons Institute
- CRT Facility
- CRT Facility Supports Collaboration with University of California at Berkeley
NERSC at Berkeley Lab provides HPC Systems for Science

- Located at Berkeley Lab
- Provides computing for a broad science community:
  - 5000 users, 700 research projects
  - 48 states; 65% from universities
  - Hundreds of users each day
  - ~1500 publications per year
- Systems designed for science:
  - 2.4PF Edison +1.3PF Hopper + .5 PF clusters
  - With services for consulting, data analysis and more
US DOE Office of Science Supercomputers at Oak Ridge, Argonne and Berkeley Labs

**Titan:**
- Peak performance of 27.1 Petaflops
- 18,688 Hybrid Compute Nodes
- 8.9 MW peak power

**Mira:**
- Peak performance of 10 Petaflops
- 49,152 Compute Nodes
- 4.8 MW peak power

**Edison XC30:**
- Peak performance 2.4PF
- 5,576 Compute Nodes
- 2.1 MW peak power
## Computing Sciences Strategy Today

<table>
<thead>
<tr>
<th>Area</th>
<th>Goal</th>
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<tbody>
<tr>
<td>Extreme Computing</td>
<td>• <strong>Goal:</strong> Increase ops/Watt by 100x</td>
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<tr>
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<td>• Hardware, software and algorithms</td>
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<td>Extreme Data</td>
<td>• <strong>Goal:</strong> Answer facility data deluge</td>
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<td>• Software, algorithms, and systems</td>
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<td>Science Engagement</td>
<td>• <strong>Goal:</strong> Improve science capabilities</td>
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<td>• Mathematics and software</td>
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<td>Computing Fundamentals</td>
<td>• <strong>Goal:</strong> Advance foundations of computing and math relevant to DOE</td>
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Applied math: broad impact from basic algorithms to scientific discovery

- **Pioneering methodology to solve previously inaccessible problems**
  - Level sets
  - Adaptive Mesh Refinement
  - High-order upwind schemes
  - Advanced eigenvalue solvers
  - Communication-avoiding algorithms

- **Software tools that enable science not previously possible**
  - Chombo, BoxLib, SuperLU, LAPACK ...

- **Broad scientific impact**
  - *climate*
  - *combustion*
  - *chemistry and materials science*
  - *cosmology*
  - *astrophysics*
  - *environmental modeling*
  - *fusion*
New numerical linear algebra techniques have impact on seismic inversion, accelerator design

- **Hsolver**: scalable HSS-embedded low-rank sparse solvers and preconditioners
  - For dense, but data-sparse structured matrices with rank-deficient off-diagonal blocks
  - Hierarchical partitioning
  - Nearly linear complexity

Sherry Li, Artem Napov, Francois-Henry Rouet, Jianlin Xia

- **ASEIG**: Algebraic sub-structuring eigensolver for $K x = \lambda M x$
  - Graph partitioning divides matrix into submatrices
  - Projection space based on eigenspectra subsets
  - Compute approximate solution from projection space
  - Advantages over Shift-Invert-Lanczos: no triangular solves, orthogonalization, less memory

Weiguo Gao, Sherry Li, Chao Yang, Zhaojun Bai
Our Strong CS Research Program at Berkeley Lab addresses the Challenge of Technology Disruption

- **Programming models and Languages**
  - Advanced programming environment addressing emerging technology challenges
  - Enable productive programming of exascale systems
  - *UPC, Titanium, DEGAS*

- **Auto-tuning and Performance Analysis**
  - Performance portability through automated runtime performance analysis and code transformations
  - *Roofline model, OSKI, X-Tune, SEJITS*

- **Communication Libraries and Resilience**
  - Addressing advanced communication facilities, error detection and recovery for future system s/w architecture
  - *GASnet, Berkeley Linux Checkpoint Restart (BLCR), CD*

- **Manycore Operating Systems and Runtimes**
  - Deconstructing the OS for manycore processors for performance isolation, error isolation, resource management
  - *K42, Tessellation, Speed Balancing*

- **Hardware Architecture and CoDesign**
  - Compiler-based automated performance model extraction and hardware simulation/simulation for ExaCT and CAL
  - *Design: Green Flash/Green Wave, View from Berkeley*
  - *Emulation: CAL, RAMP*
Data in Bioinformatics Requires New Algorithms, Software, and Systems

Sequencing Cost Drops Again

Gene Context Analysis now >1000x faster using FastBit

Strong Scaling of Meraculous Assembler in UPC

Probabilistic counting, Bloom filters, Distributed hash

New ~Linear Time Bubble Clustering algorithm

Human: 2B reads → 20M contigs → 16K scaffolds → 23 chromosomes

A. Buluc, V. Strnadova. J. Gilbert, E. Georganas, J. Chapmanz, D. Rokhsar, L. Olier, and K. Yelick., multiple papers to be submitted
Expansion of Computational Science at Berkeley Lab driven by challenges of data-intensive experiments and observations

• We have a strong record of innovation in computational science, mostly modeling and simulation
  – Major SciDAC role – including climate, astrophysics
  – Outstanding applied math
  – Visionary computer science
  – Lead DOE’s data intensive computing center SDAV
  – NERSC and ESnet are major DOE computational facilities

• But our science facilities are largely experimental in nature – data analysis has not been an HPC problem*

• Exploding data intensive analysis demands means opportunity for significant growth in computing for science at LBNL
  – Beamline data
  – Materials discovery - database approaches
  – Bio-image analysis
  – Genomics data - JGI
  – Modeling and Simulation to help understand observations – e.g. cosmology

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* Possibly excluding JGI
Data Growth is Outpacing Computing Growth

Graph based on average growth

Projected Data Rates Relative to 2010

- Detector
- Sequencer
- Processor
- Memory

Data-driven scientific discovery requires integration of modeling, simulation, analysis, data management

**Example: 21st Century Astrophysics:**

– Tight collaboration between astrophysicists and computational scientists to develop new technologies for cosmological data analysis

– Analysis & simulation of 100s of TeraBytes of data from ground- and space-based observations

– Modeling & simulation of supernovae and large-scale structure formation
Advanced analytic techniques needed to identify interesting events in climate data

- New data mining, image processing, and topological analysis techniques
- Detect extreme events, e.g., hurricanes
- 10s-100s of TB of data from a single simulation
  - (The Library of Congress contains about 254 TB.)
- TECA Toolkit
  - Automatic detection of cyclones, atmospheric rivers, and more
  - Analysis time years to minutes

High-resolution atmospheric simulation

Detected cyclones
CAMERA leverages state-of-the-art mathematics to transform experimental data into understanding.

**CENTER FOR APPLIED MATHEMATICS FOR ENERGY RESEARCH APPLICATIONS**

- **X-ray scattering data analysis**
  - HipGISAXS
  - 400-1500x faster analysis for X-ray scattering data
  - **Now:** Nonlinear optimization, genetic algorithms, pattern recognition w/ noise

- **Micro-CT Sample Analysis**
  - Quant-CT provides automated quantitative analysis
  - **Now:** 3D image segmentation; pattern recognition; classification; PDE- and graph-based analysis

- **X-ray Nano-Crystallographic Reconstruction**
  - Indexing ambiguity resolved [PNAS13]
  - **Now:** Image orientation, find crystal shape/size; address orientation ambiguities; data variance reduction

- **Designing New Materials**
  - Designed record-breaking high-surface area materials
  - **Now:** 3D porous polymer model assembly; Zeo++ porosity characterization; Optimal material designs

**LDRD-seeded, now ASCR-supported**

**U.S. DEPARTMENT OF ENERGY**

Sherry Li, D. Ushizima, J. Donatelli, M. Haranczyk, J. Sethian
Robust software infrastructure for modern scientific discovery

• **ATLAS (CERN):** LBNL responsible for core software and infrastructure (since 1999) – 8 FTE effort

• **Daya Bay:** LBNL architected software for anti-neutrino mixing angle experiment (2012)

• **Data servers supporting users and analysis**
  - FLUXNET carbon flux measurement
  - National Soil Carbon Network
  - Advanced Simulation Capabilities for Environmental Management
  - Carbon Capture Simulation Initiative
  - Materials Genome Database
SPOT Suite: New Usage Model for Light Sources

• Light source data solution:
  – Data management and storage
  – Analysis and simulation

• Inter-disciplinary team:
  – Computer scientists
  – Light source scientists
  – Materials scientists
  – ESNet & NERSC

• In-situ, time-resolved experiments,
• Real-time analysis, algorithms,
• Data sharing & collaboration

Since March 2013: 40 experiments; 1,356 datasets; 16 TB of raw data; 346,371 NERSC jobs delivered in real time to BL 8.3.2 Micro-Tomography Beamline.

Craig Tull, Alexander Hexemer, Dula Parkinson
Tigres provides programming templates for developing scientific workflow pipelines

- **Science targets:**
  - Image processing
  - Light source experiments
  - Cosmology
  - DNA assembly
  - UQ pipelines

- **Design Goals:**
  - Easy composition
  - Scalability
  - Lightweight execution

- **Templates:**
  - Sequence
  - Parallel
  - Split
  - Merge
We hope to identify collaboration opportunities between Berkeley Lab and CCS during this meeting

- **Michael Wehner**: Simulating Hurricanes and Typhoons in a Global Climate Model
- **Esmond Ng**: Large-scale Eigenvalue Calculations in Scientific Applications
- **Costin Iancu**: Dynamic Exascale Global Address Space (DEGAS) Programming Environments
- **Casey Stark**: The Lyman-alpha Forest in Cosmological Hydrodynamic Simulations
- **Khalid Ibrahim**: Analysis and Optimization of Gyrokinetic Toroidal Simulation on Emerging Architectures