My facility had an anniversary last year too!
There’s something magical that happens at 50. It’s an age where experience meets opportunity, wisdom intertwines with energy, and life takes on a new vibrancy.

Alex Mustaros on Medium
Lethal Dose: 1 nanosecond
• Managers
• Scientists
• Administrators
• Communications
• Business management
• Project management
• Facility management
• Logistics

• Accelerator operations
• Radiation safety
• Chemical safety
• Biological safety
• Mechanical engineering
• Survey and Alignment
• Vacuum systems
• Mechanical technology

• Electrical engineering
• Electronics maintenance
• Electronics installation
• Electricians
• Controls
• IT/Network
• Data Science
• Computing

TEAM SCIENCE
1000s of USERS from many science domains
I saw computing taking an increasing % of users’ time
Thanks to Dani Ushizima for telling me in 2010 about how I could use NERSC to help!

Dula Parkinson <DYParkinson@lbl.gov> Tue, Nov 30, 2010, 3:44 PM

to Alastair ▼

A "portal" to NERSC was what Dani suggested when I told her we wanted a window on our data after some of it is processed, without having to transfer the whole data set back and forth.
Creating Super-Facilities - a Coupled Facility Model for Data-Intensive Science

Craig E. Tull, PhD
LBNL Computing Research Division

- Multi-ASCR Facility Demos hint at the power of a BES-ASCR "Super-facility" to dramatically advance science.

CETull@lbl.gov - 08 October 2014
Data Rate Analysis for Esnet Requirements Review 2014: “You don’t belong”

ALS Case Study for ESnet Network Requirements Review, September 2014
Please scroll down to see assumptions and explanations

Include: All beamlines
Sort beamlines by: Overall Ave

Include: Only Current Beamlines
LAN: Current
WAN: Current
Detectors: Current Increase readouts by 2 x
ALS/Optics: Current Decrease exposure by 10 x
Sample Automation: Current Decrease sample change by 5 x

Based on current settings, calculated rates are:
Max: 7.24Gbps (25.33 PB/year)
Operating Average: 0.79Gbps (2.76 PB/year)
Overall Average: 0.40Gbps (1.39 PB/year)

<table>
<thead>
<tr>
<th>Beaml ine</th>
<th>Exposure</th>
<th>Detector</th>
<th>LAN</th>
<th>WAN</th>
<th>Overall Max</th>
<th>Ave During Ops</th>
<th>Overall Ave</th>
<th>TB per Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.2.2, TousM1L</td>
<td>2.35</td>
<td>2.65</td>
<td>10.00</td>
<td>10.00</td>
<td>0.25</td>
<td>0.24</td>
<td>0.87</td>
<td>241.41 TB/yr</td>
</tr>
<tr>
<td>4.2.2, MAD-MX</td>
<td>2.33</td>
<td>2.33</td>
<td>10.00</td>
<td>10.00</td>
<td>0.30</td>
<td>0.20</td>
<td>0.06</td>
<td>222.53 TB/yr</td>
</tr>
<tr>
<td>5.0.3, BC58-PX</td>
<td>0.30</td>
<td>0.30</td>
<td>10.00</td>
<td>10.00</td>
<td>0.20</td>
<td>0.20</td>
<td>0.04</td>
<td>132.40 TB/yr</td>
</tr>
<tr>
<td>5.0.2, BC58-PX</td>
<td>0.30</td>
<td>0.30</td>
<td>10.00</td>
<td>10.00</td>
<td>0.20</td>
<td>0.20</td>
<td>0.04</td>
<td>132.40 TB/yr</td>
</tr>
</tbody>
</table>

BERKELEY LAB

12
2023 Scientific: The Superfacility Team: William Arndt, Debbie Bard, Johannes Blaschke, Shane Canon, Ravi Cheema, Shreyas Cholia, Bjoern Enders, Lisa Gerhardt, Annette Greiner, Chin Guok, Damian Hazen, Doug Jacobsen, Stefan Lasiewski, Jason Lee, Kelly Rowland, Chris Samuel, Ashwin Selvarajan, Alex Sim, David Skinner, Cory Snavely, Laurie Stephey, Rollin Thomas, Gabor Torok, Becci Totzke, Xi Yang

Citation: For developing and demonstrating the revolutionary Superfacility concept, coupling high performance computing, networking, services and tools with a range of experimental and observational science facilities spanning multiple science domains.
Welcome Dilworth Y. Parkinson

Important Log In and Links Information for Users

New users: Create an account by logging in using one of the login options (we encourage using LBNL Single Sign On). You will need to complete the mandatory safety training

Your Status

Access Status

LBNL#: 005481
Appointment Status: Active
Appointment Start/End Dates: 07/07/2010 -
LBNL Badge status: Active
Badge Expiration Date: 07/11/2024
ALS Remote access: Active
General required on-site training complete: Yes

Safety Training (Do not do without an LBNL#)

LBNL # is issued in Human Resources welcome email
The Super Facility Isn’t Just a Demo!
What is NERSC?

- hardware, software, documentation, and PEOPLE
- high performance
- data
- open and accessible
- remotely access
- impact on science across domains
- collaboration enabler
What is the impact of NERSC?

• NERSC means that synchrotron newbies like me can immediately jump in and start visualizing and analyzing data, and worry about becoming an expert once we're ready for the next step.

• NERSC allows us to quickly search, visualize, and process a large catalog of data spanning over 10 years of active research at LBNL.
NERSC is a Supercomputer with a Heart
5. Kas Anderle
Developing next generation microchips with nano-scale lithography
Finite-Element (FE) Maxwell solver Calculations to support X-ray Scattering

- Filling the shape with FE
- Calculating the E-Field distribution for a specific angle of incidence and energy and then calculating the intensity in the diffraction orders
- Using an optimization method to find the shape that describes the experimental data the best (solving an inverse problem)
4. Hasitha Wijesuriya
Sand in earthquakes

UC Berkeley
Advisor Nick Sitar
From sample collection to simulation

Sample Collection
(diameter - 11 mm, length – 22 mm)

Triaxial compression test with flexible membrane

TX testing @ Beamline 8.3.2 – ALS, LBNL

Reconstructed grains
(# grains – 80,000 – 100,000)

Grain Reconstruction

Scanning

DEM Simulation

Setup
3. Kanupriya Pande: High resolution tomography image alignment
Alignment of X-ray Tomography

- Joint 3D rigid-body alignment and reconstruction
- Python frontend with Fortran projectors
- openMP + MPI for parallelization
- Bayesian optimization for tilt of axis and COR

\[ f^k = \arg \min_f \left\{ \frac{1}{2} \| A(\Theta^{k-1}) f - p \|_2^2 + \lambda R(f) \right\} \]  
**SIRT, CG, FISTA**

\[ \Theta^k = \arg \min_\Theta \left\{ \frac{1}{2} \| A(\Theta) f^k - p \|_2^2 + \gamma G(\Theta) \right\} \]  
**GD, Quasi-Newton**

\[ A(\Theta)f = \sum_j \sum_{x_g} f(x_g)k(p_j - x_g) \]  
**Trilinear, Cubic Spline**

\[ \nabla_\Theta A(\Theta)f = \sum_j \sum_{x_g} f(x_g) \frac{\partial p_j}{\partial \Theta} \cdot (\nabla k(p_j - x_g))^T \]  
**Analytical derivatives**

\[ \nabla_\Theta A(\Theta)f = \sum_j \sum_{x_g} f(x_g) \frac{\partial p_j}{\partial \Theta} \cdot (\nabla k(p_j - x_g))^T \]  
**Analytical derivatives**

In collaboration with H. Yan at NSLS II

Pande, Donatelli, Parkinson, Yan, Sethian, Optics Express (2021)
2. Gustavo Zottis Girotto
• Placement of adatoms on AB-stacked graphene and observation of transition states
• Performing Ab initio molecular dynamics
• using Quantum ESPRESSO 7.1 on NERSC under ALS account
• Multiple parallel jobs, 1 or 2 nodes each, 128 cores per CPU node, 2 threads per process
• Complementary to work performed on beamlines 11.0.2, 9.3.2 and 9.0.1
• See preprint: https://doi.org/10.26434/chemrxiv-2024-r6mw7
1. Benjamin Ringel: Spacecraft heat shields
Data acquired at SLS TOMCAT beamline in high temperature cell. Data reconstructed with custom tomopy script on NERSC supercomputer. Segmentation using deep learning models with ORS Dragonfly. Binary data used to measure time resolved properties of material. Data analysis process requires managing over 30TB of data!
Porosity

**Diffusion-Limited**
- Power: 18 A
- Temp.: 1320 K
- Pressure: 100.5 kPa

**Mixed Regime**
- Power: 15 A
- Temp.: 1060 K
- Pressure: 100.0 kPa

**Reaction-Limited**
- Power: 13 A
- Temp.: 945 K
- Pressure: 100.7 kPa

Graph showing depth as a function of porosity for each regime.
PuMA Property Computation

**Material orientation.** *Computational Materials Science* (2020)

**Effective conductivity.** *Computational Materials Science* (2021)

**Effective elasticity.** *AIAA SciTech Forum* (2022)

**Effective permeability.** *Computational Materials Science* (2023)
Simulation/Experiment Comparison

![Graph showing comparison between simulation and experiment for oxidation depth as a function of normalized time. The graph includes lines for different temperatures (T = 1320 K, T = 1060 K, T = 945 K) and distinguishes between experiment (solid line) and simulation (dotted line).]
We’re living in the future!
More Intuitive Supercomputing
KAIAA (Kind AI At ALS)

• (for people looking at these shared slides, see script in the notes below)
Thanks!

- ALS
- NERSC
- ESnet
- IT
- Computing Sciences

- DOE BES
- DOE ASCR

- And many more!
There’s something magical that happens at 50. It’s an age where experience meets opportunity, wisdom intertwines with energy, and life takes on a new vibrancy.

Alex Mustaros on Medium