Intuitive Supercomputing for X-rayers

Dula Parkinson

Advanced Light Source
Lawrence Berkeley National Laboratory

June 2024

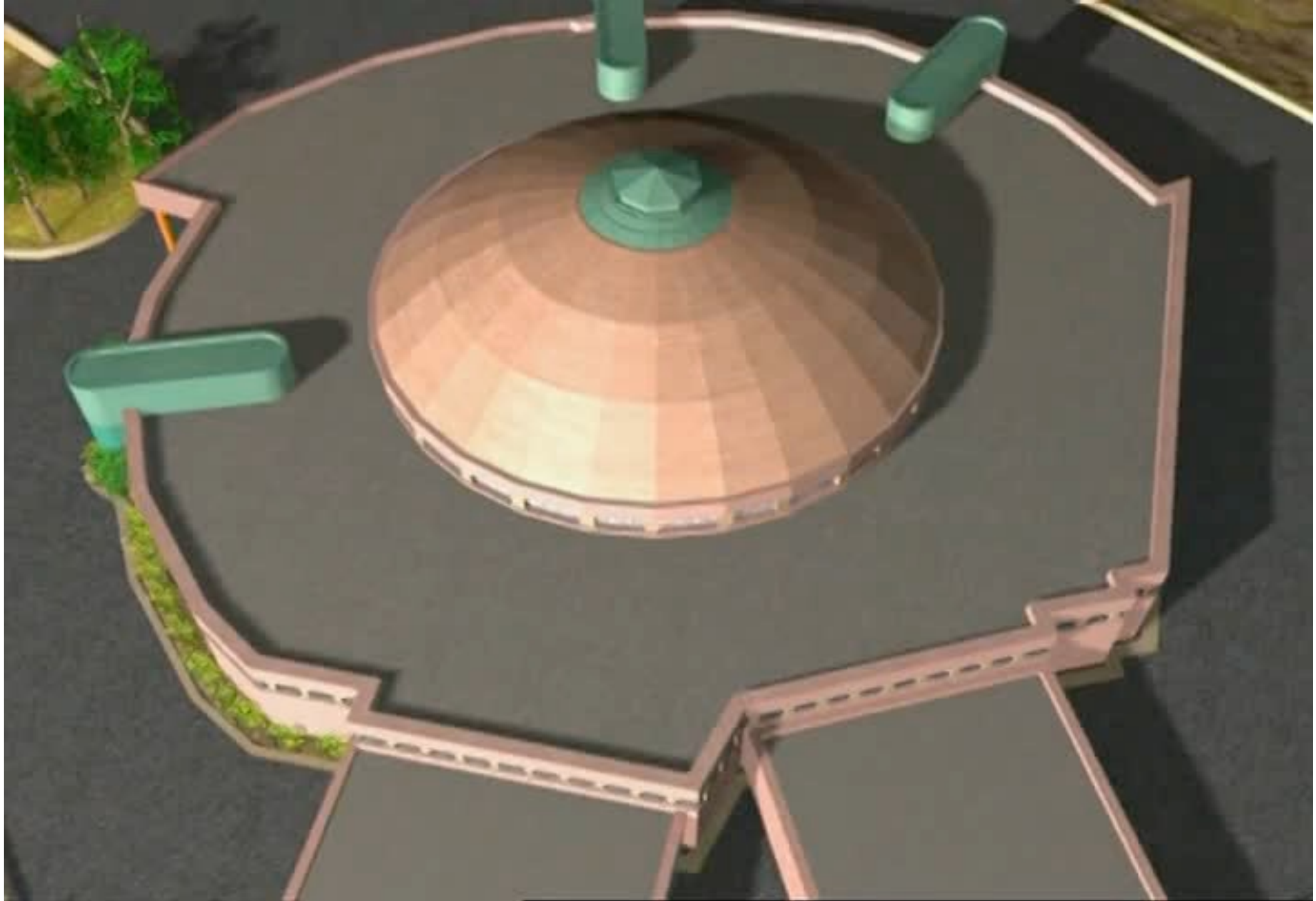
My facility had an anniversary last year too!

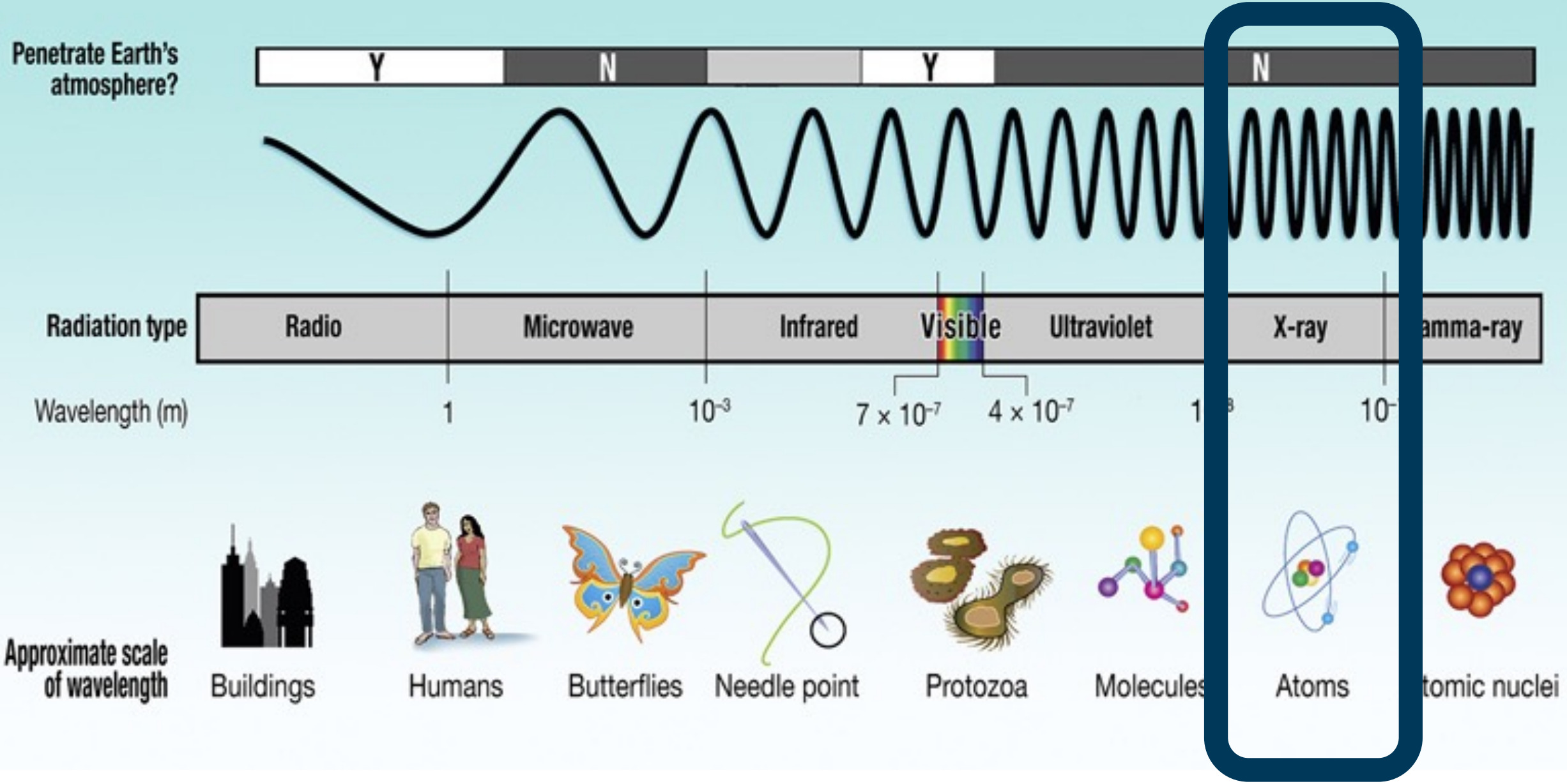
NERSC@50 | SEMINAR | SERIES

“Turning 50 today feels like what turning 30 used to”

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



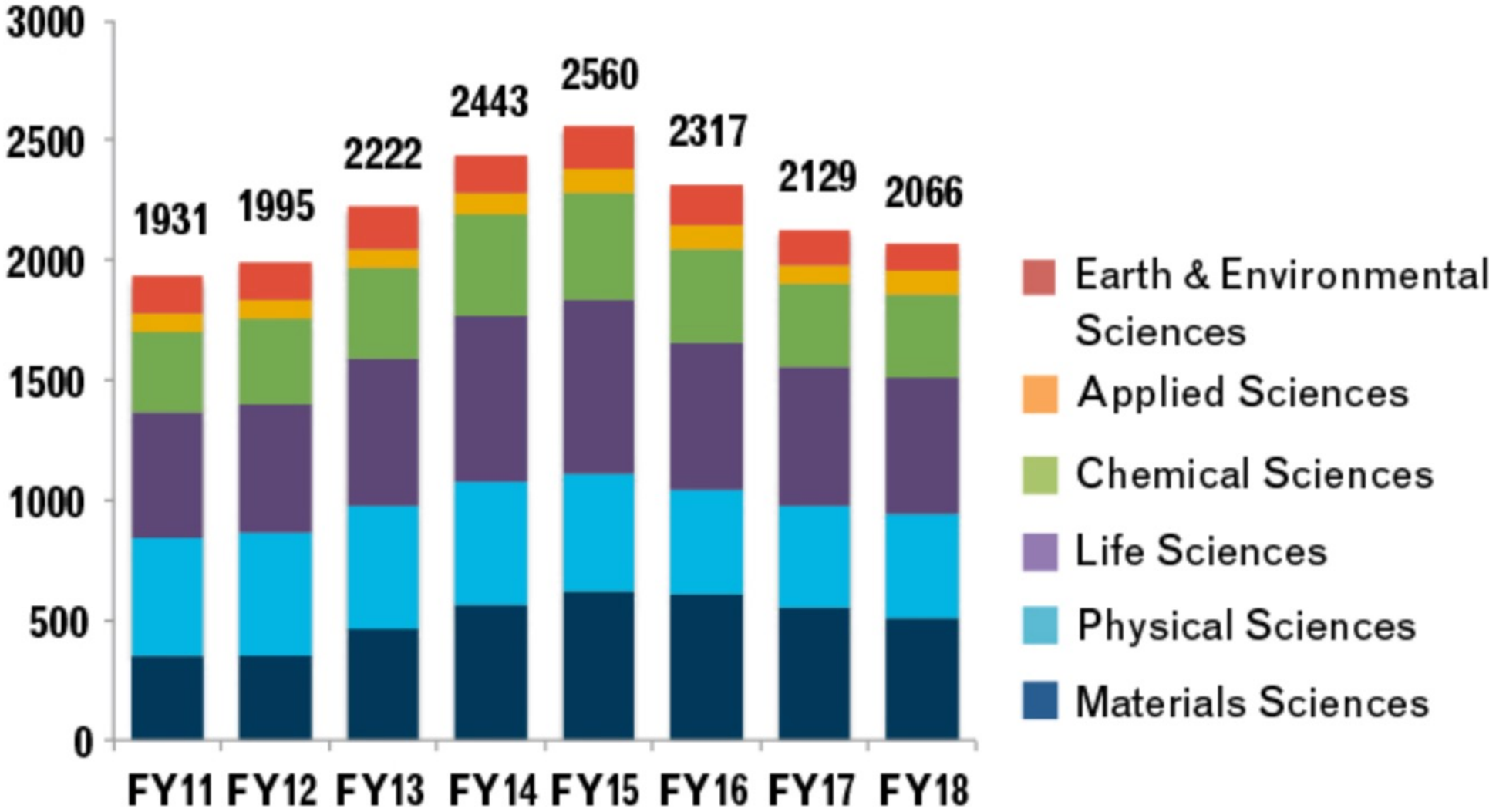

Penetrate Earth's atmosphere?
Y
N
Y
N
Radiation type
Radio
Microwave
Infrared
Visible
Ultraviolet
X-ray
amma-ray
Wavelength (m)
1
10⁻³
7 x 10⁻⁷
4 x 10⁻⁷
10⁻
Approximate scale of wavelength
Buildings
Humans
Butterflies
Needle point
Protozoa
Molecules
Atoms
tomic nuclei


Lethal Dose:
1 nanosecond

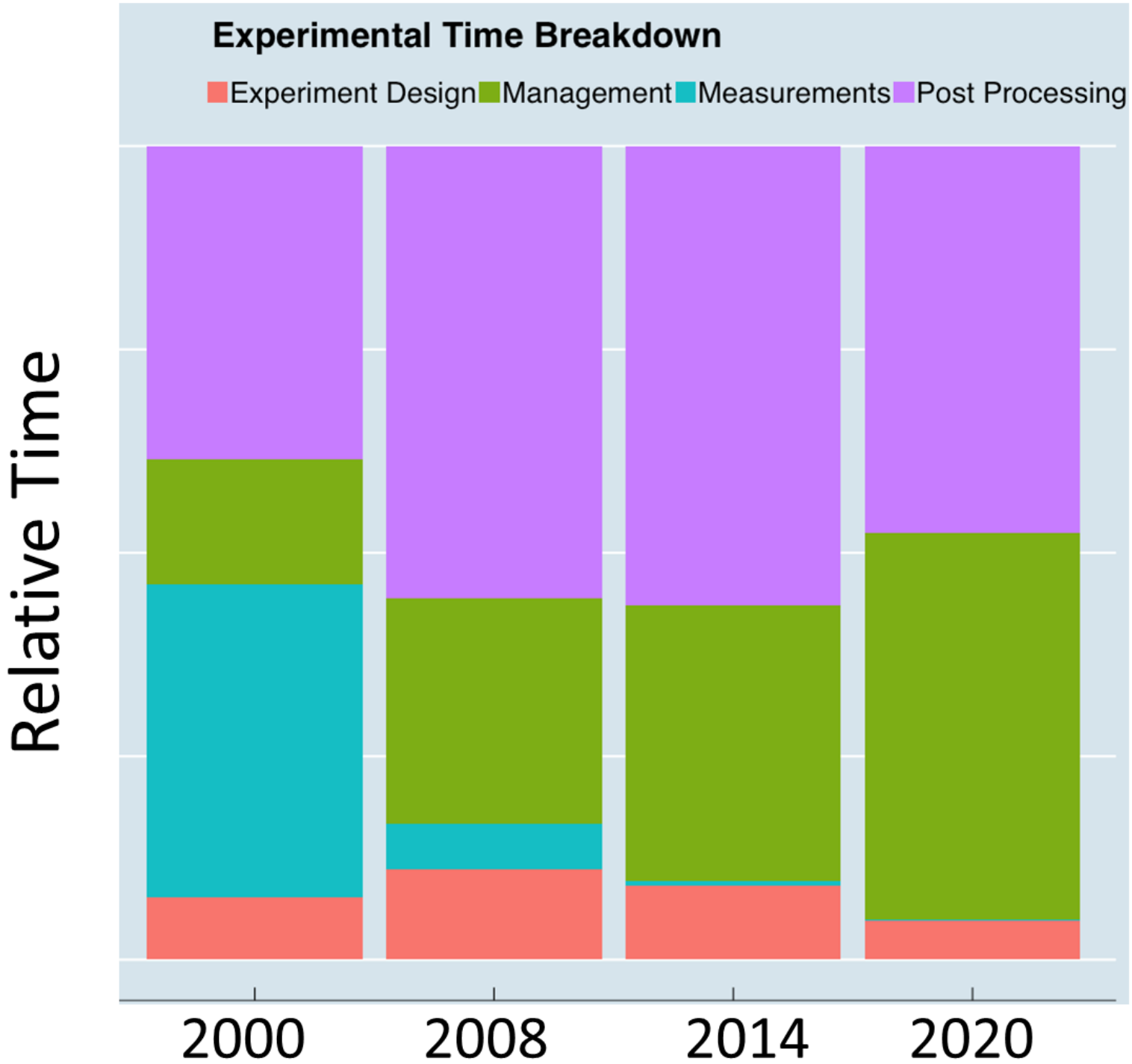
- Managers
- Scientists
- Administrators
- Communications
- Business management
- Project management
- Facility management
- Logistics
- Accelerator operations
- Radiation safety
- Chemical safety
- Biological safety
- Mechanical engineering
- Survey and Alignment
- Vacuum systems
- Mechanical technology
- 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.

•••

BERKELEY LAB
LAWRENCE BERKELEY NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

SPOT

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

BERKELEY LAB
LAWRENCE BERKELEY NATIONAL LABORATORY

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 ▾

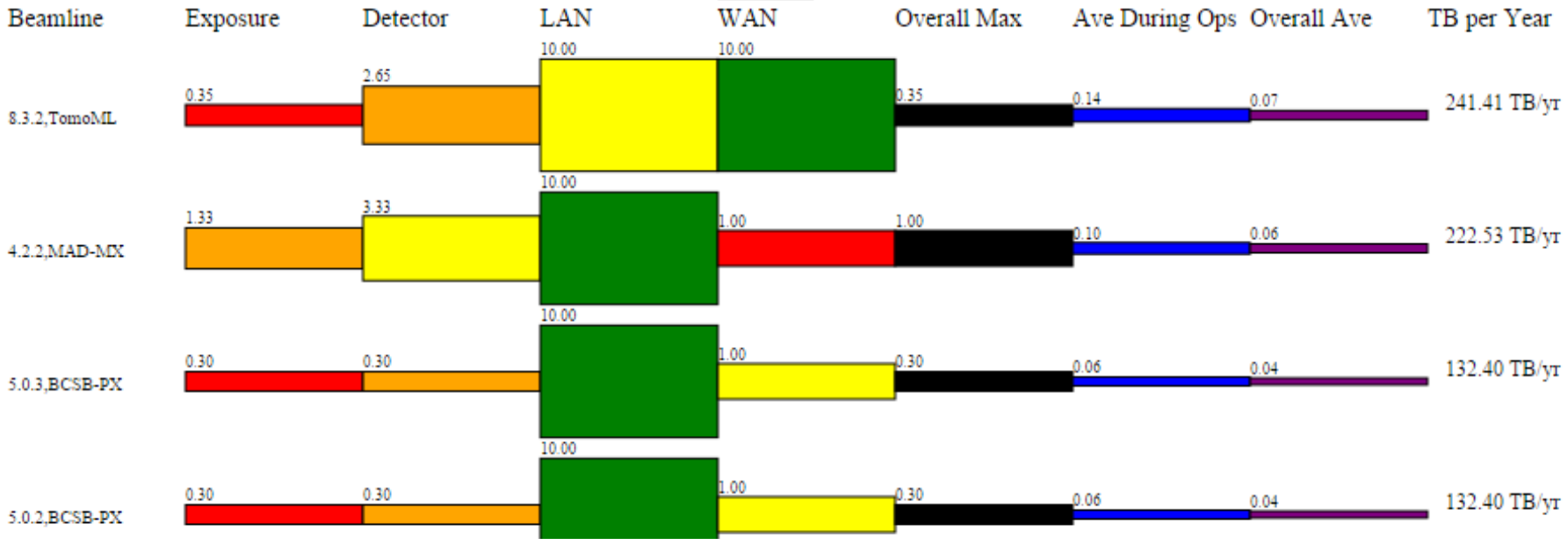
Include: Only Current Beamlines ▾
LAN: Current ▾
WAN: Current ▾
Detectors: Current ▾ Increase readouts by 2 x
ALS/Optics: Current ▾ Decrease exposure by 10 x
Sample Automation: Current ▾ Decrease sample change by 5 x

Based on current settings, calculated rates are:

Max: 7.24Gbps (25.33 PB/year)

Operating Average: 0.79Gbps (2.76 PB/year)

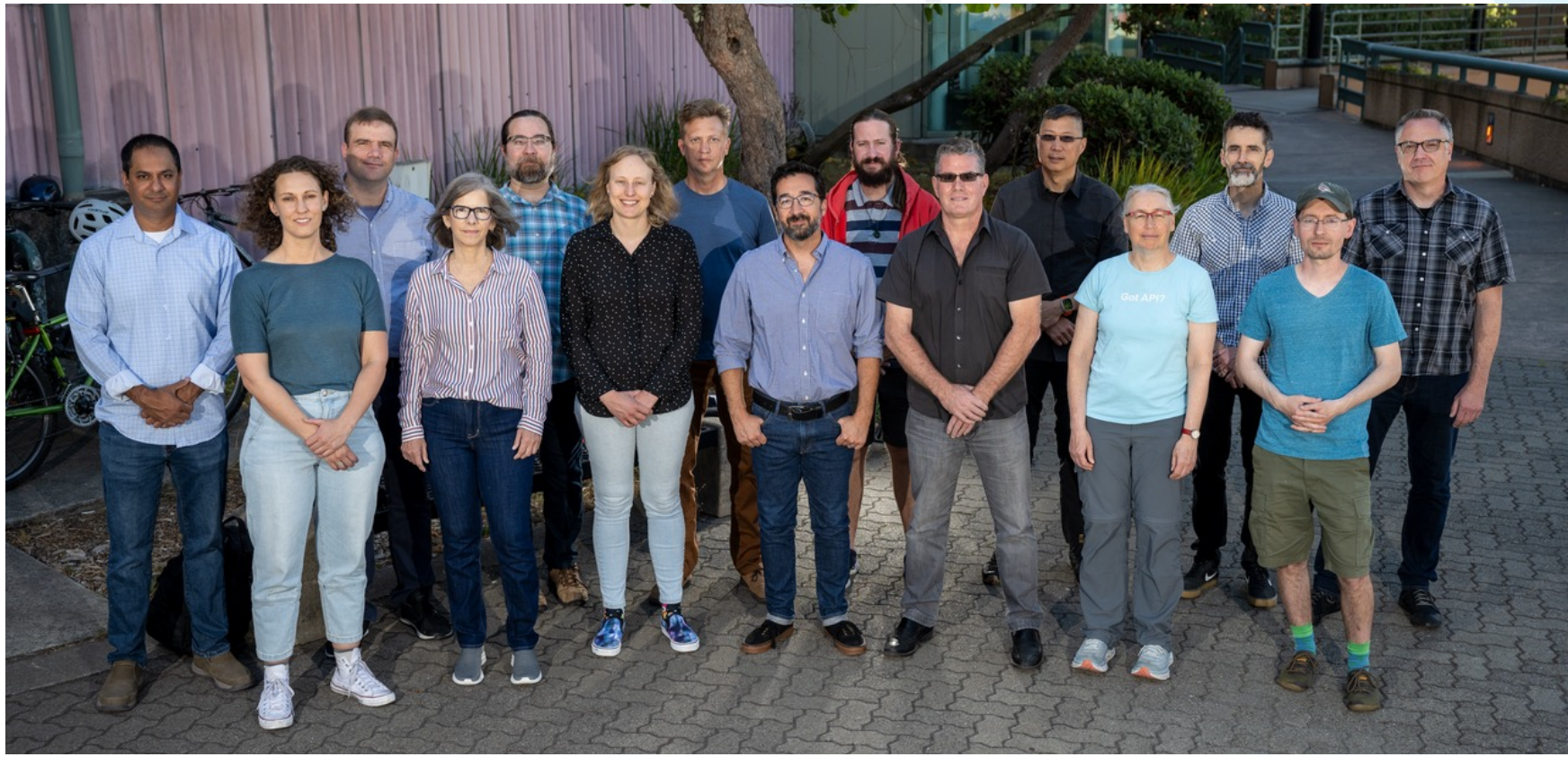
Overall Average: 0.40Gbps (1.39 PB/year)



2023 LBNL Director's Award for Scientific Achievement: The Superfacility Team

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.*



ALSHub

BERKELEY LAB

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

Your Status

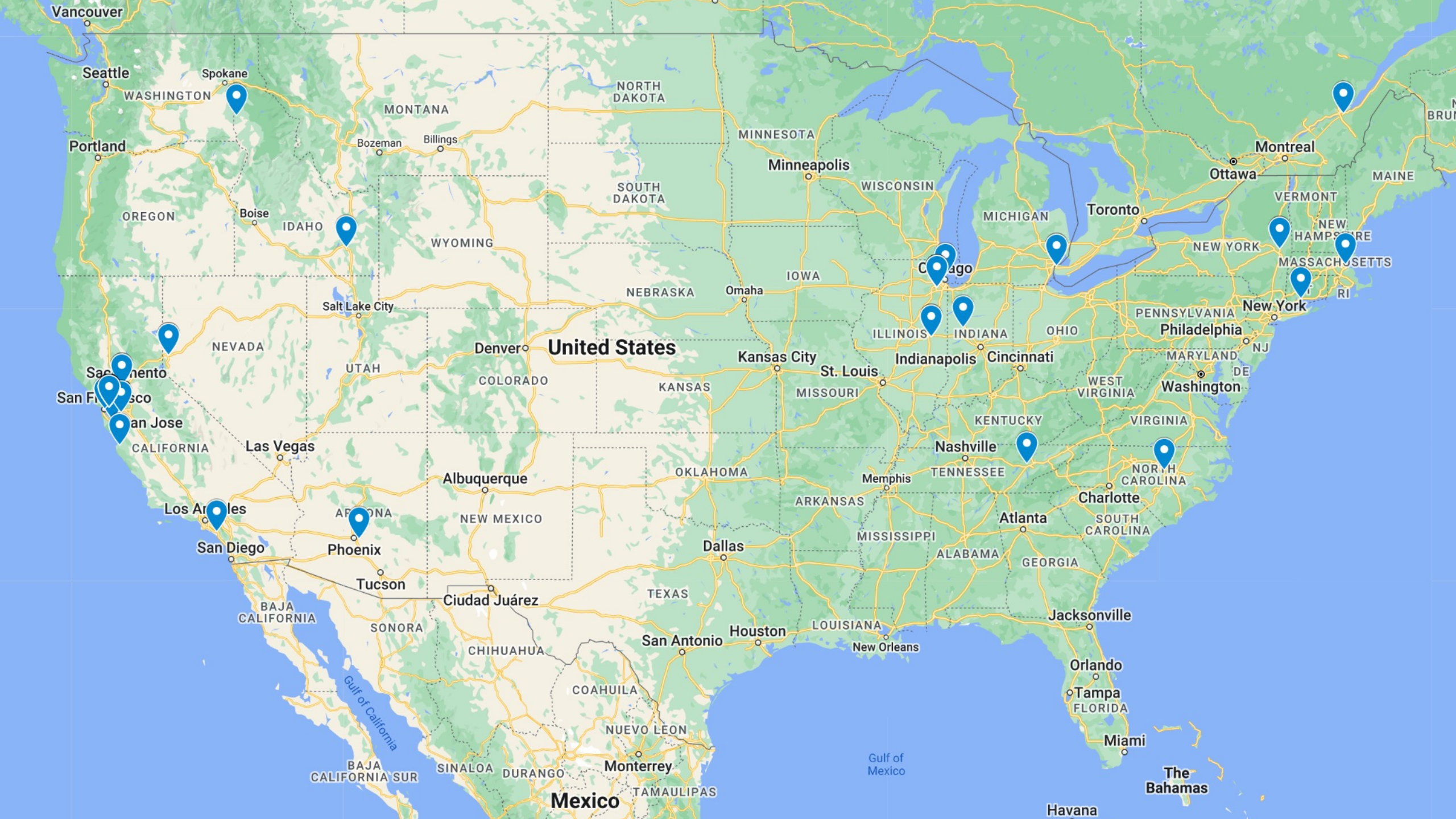
Access Status
LBNL#:**005481**
Appointment Status: ✓ Active
Appointment Start/End Dates:
07/07/2010 -
LBNL Badge status: ✓ Active
Badge Expiration Date: 07/11/2024
ALS Remote access: ✓ Active
General required on-site training complete: Yes

Arrival Timeline
Your requested arrival date: Update
None

User Agreement
Non-proprietary: Expires 12/31/2099
Proprietary: None

Safety Training (Do not do without an LBNL#)
LBNL # is issued in Human Resources welcome email

The Super Facililty Isn’t Just a Demo!


Vancouver
Seattle
Spokane
WASHINGTON
Portland
MONTANA
Bozeman
Billings
NORTH DAKOTA
MINNESOTA
Minneapolis
SOUTH DAKOTA
WISCONSIN
Montreal
Ottawa
MAINE
VERMONT
OREGON
Boise
IDAHO
WYOMING
MICHIGAN
Toronto
NEW HAMPSHIRE
NEW YORK
MASSACHUSETTS
RI
IOWA
NEBRASKA
Omaha
Salt Lake City
NEVADA
UTAH
Denver
United States
COLORADO
Kansas City
St. Louis
KANSAS
MISSOURI
ILLINOIS
INDIANA
OHIO
Indianapolis
Cincinnati
PENNSYLVANIA
New York
Philadelphia
NJ
MARYLAND
DE
WEST VIRGINIA
Washington
KENTUCKY
VIRGINIA
Nashville
TENNESSEE
Memphis
NORTH CAROLINA
Charlotte
Atlanta
SOUTH CAROLINA
ARKANSAS
MISSISSIPPI
ALABAMA
GEORGIA
Albuquerque
OKLAHOMA
NEW MEXICO
Las Vegas
CALIFORNIA
San Jose
Los Angeles
San Diego
Phoenix
Tucson
Dallas
TEXAS
Ciudad Juárez
BAJA CALIFORNIA
SONORA
CHIHUAHUA
Houston
San Antonio
LOUISIANA
New Orleans
Jacksonville
Orlando
Tampa
FLORIDA
Miami
COAHUILA
NUEVO LEON
Monterrey
TAMAULIPAS
SINALOA
DURANGO
BAJA CALIFORNIA SUR
Gulf of California
Gulf of Mexico
Mexico
The Bahamas
Havana

What is NERSC?

- hardware, software, documentation, and PEOPLE
- high performance
- data
- open and accessible
- remotely access
- impact on science across domains
- collaboration enabler

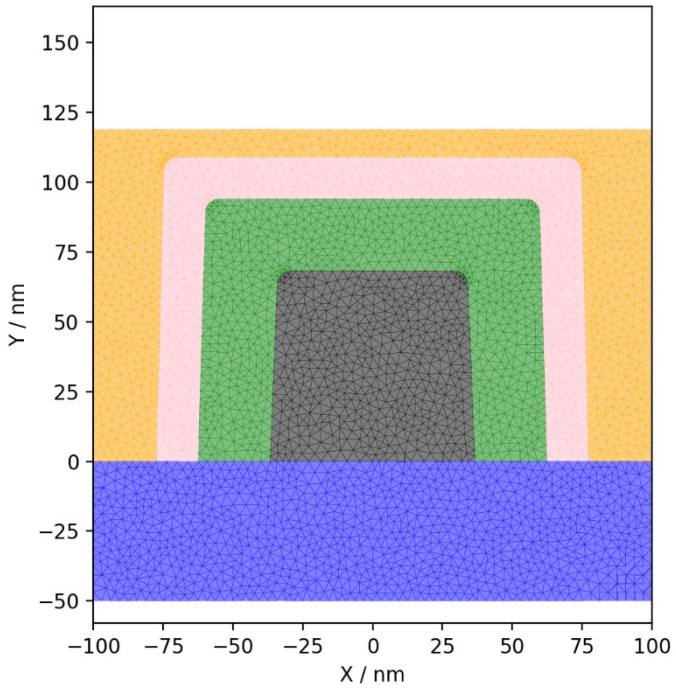
What is the impact of NERSC?

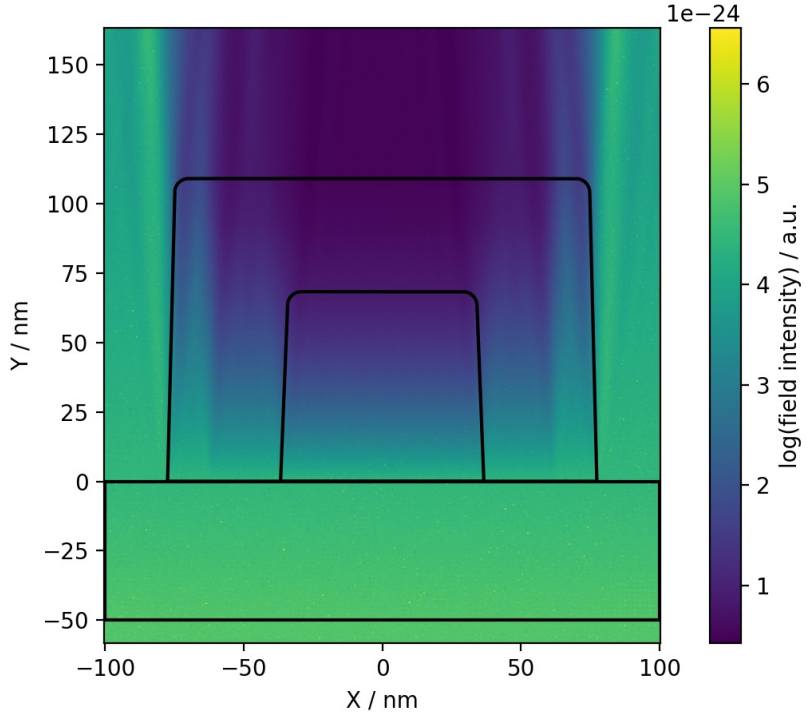
- NERSC means that synchrotron newbies like me can immediately jump in and start visualizing and analyzing data, and worry about becoming an expert once we're ready for the next step
- NERSC allows us to quickly search, visualize, and process a large catalog of data spanning over 10 years of active research at LBNL

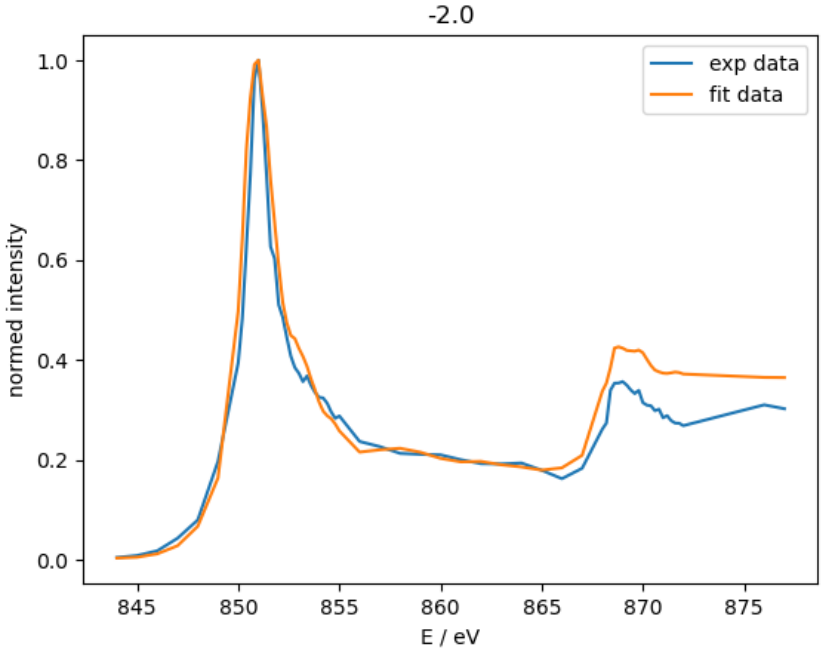
NERSC is a Supercomputer with a Heart

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 than 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)

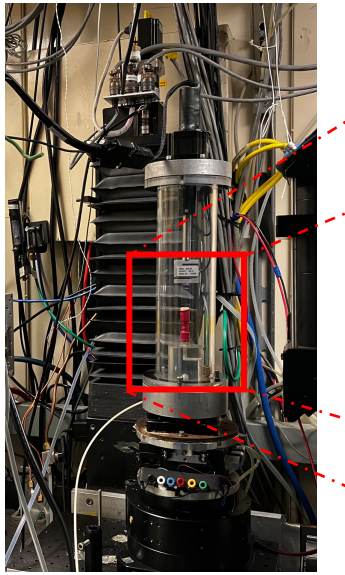
4. Hasitha Wijesuriya
Sand in earthquakes

UC Berkeley
Advisor Nick Sitar

From sample collection to simulation

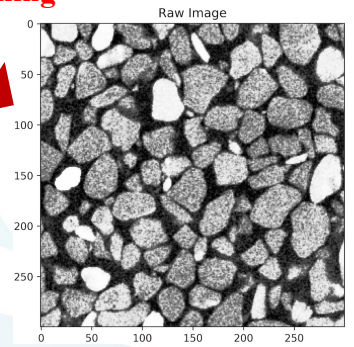
Sample Collection
(diameter - 11 mm,
length – 22 mm)

Setup

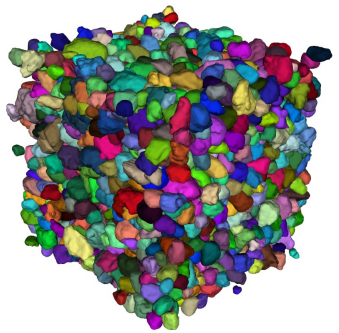


TX testing @ Beamline 8.3.2 –
ALS, LBNL

Scanning



Grain
Reconstruction



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

DEM
Simulation

Triaxial compression test with flexible membrane

3. Kanupriya Pande: High resolution tomography image alignment

Alignment of X-ray Tomography

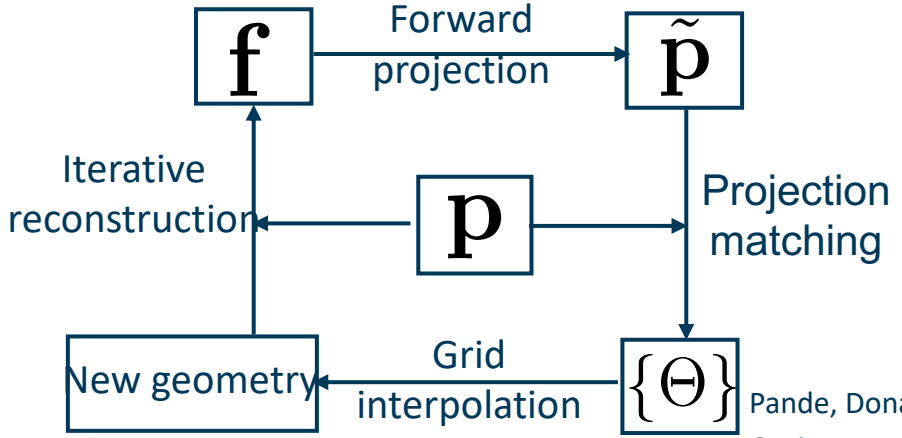
- Joint 3D rigid-body alignment and reconstruction
- Python frontend with Fortran projectors
- openMP + MPI for parallelization
- Bayesian optimization for tilt of axis and COR

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

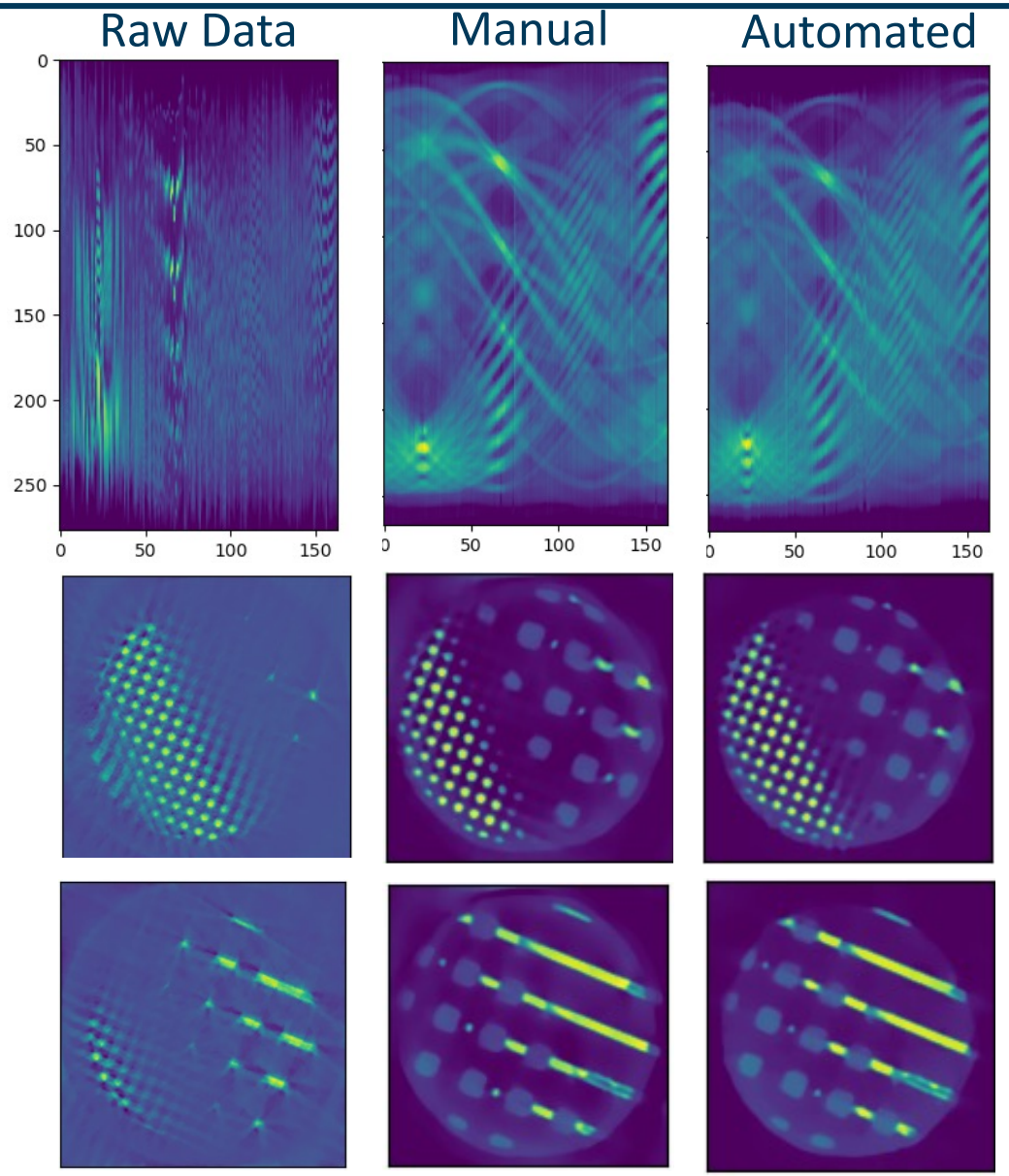
$$\Theta^k = \arg\min_\Theta \left\{ \frac{1}{2} \| A(\Theta) f^k - p \|_2^2 + \gamma G(\Theta) \right\}$$ **GD, Quasi-Newton**

$$A(\Theta) f = \sum_j \sum_{\mathbf{x}_g} f(\mathbf{x}_g) k(\mathbf{p}_j - \mathbf{x}_g)$$ **Trilinear, Cubic Spline**

$$\nabla_\Theta A(\Theta) f = \sum_j \sum_{\mathbf{x}_g} f(\mathbf{x}_g) \frac{\partial \mathbf{p}_j}{\partial \Theta} \cdot (\nabla k(\mathbf{p}_j - \mathbf{x}_g))^T$$ **Analytical derivatives**



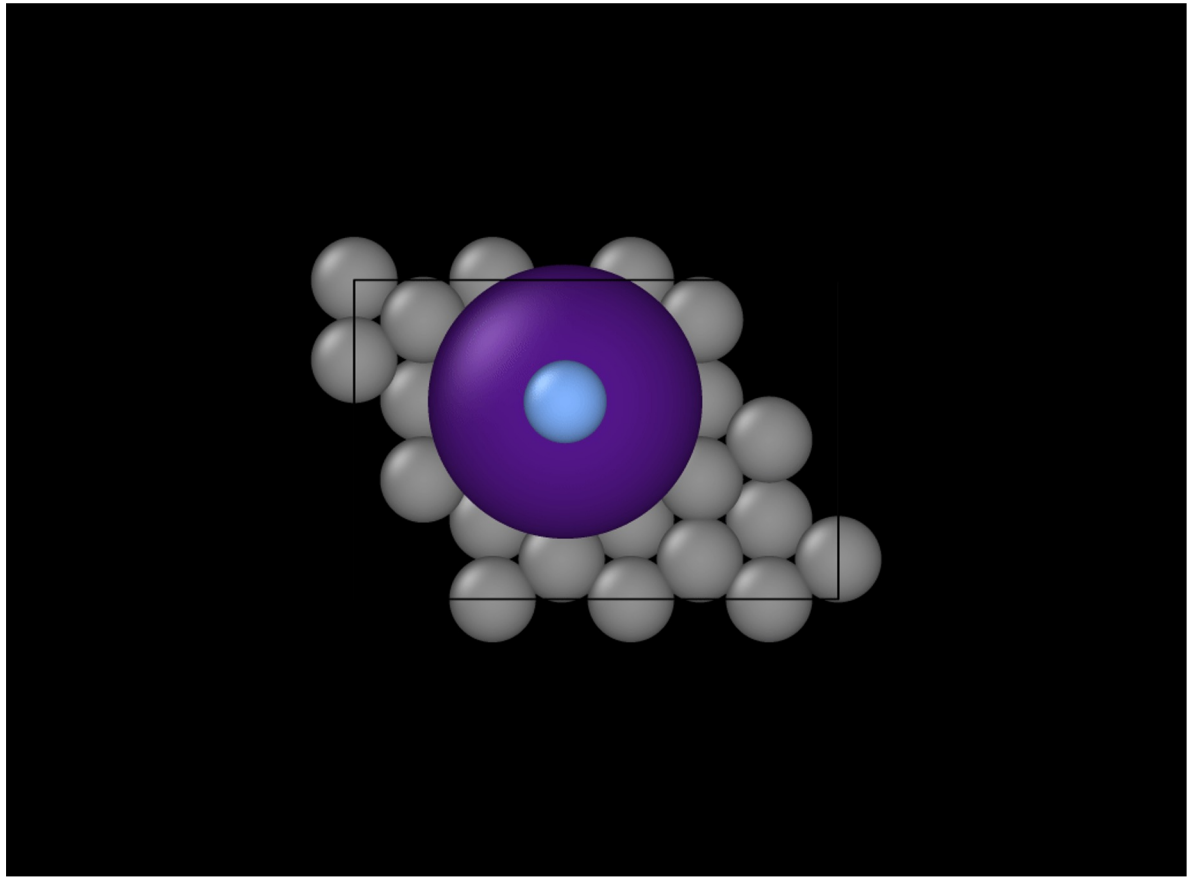
Pande, Donatelli, Parkinson, Yan, Sethian, Optics Express (2021)



In collaboration with H. Yan at NSLS II

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

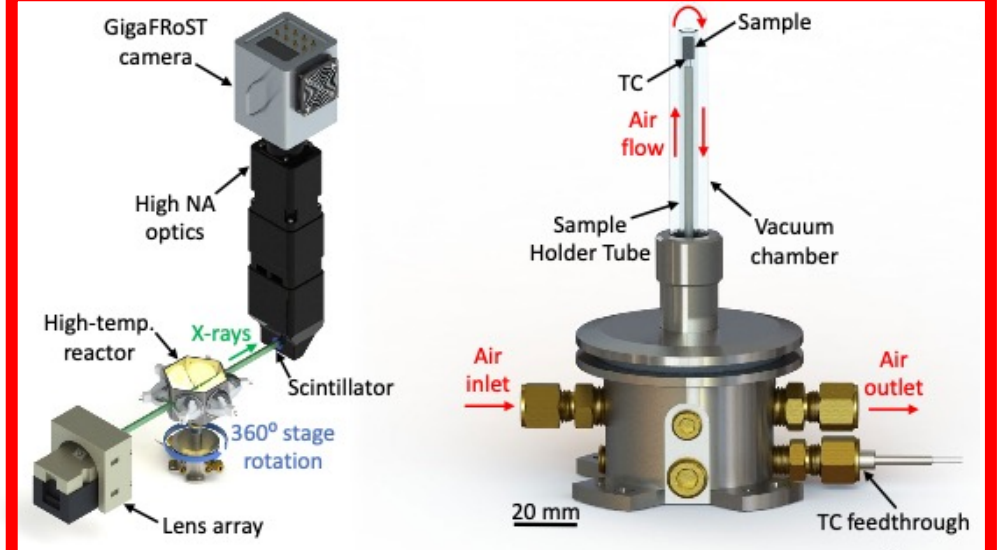


Benjamin Ringel[a], Federico Semeraro[b], Joseph Ferguson[c], Bruno Dias[b], Harold Barnard[d], Dilworth Parkinson[d], Francesco Panerai[a]

[a]Center for Hypersonics & Entry System Studies, Department of Aerospace Engineering, University of Illinois at Urbana-Champaign, Urbana, IL
[b]Analytical Mechanics Associates, NASA Ames Research Center, Moffett Field, CA
[c]Department of Mechanical Engineering, Stanford University, Stanford, CA
[d]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA

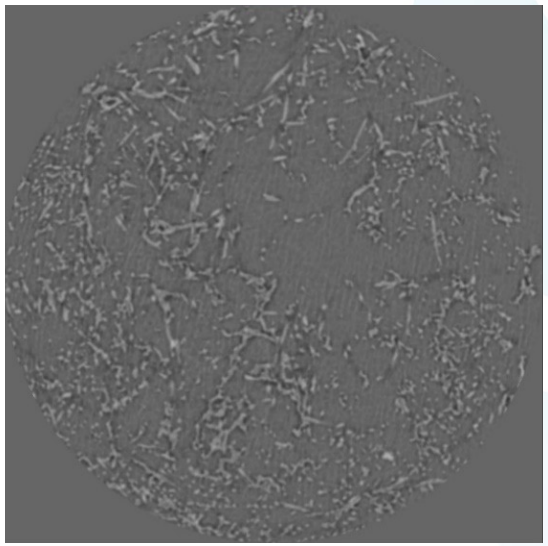
1. Benjamin Ringel: Spacecraft heat shields

4D Micro-CT Data Process

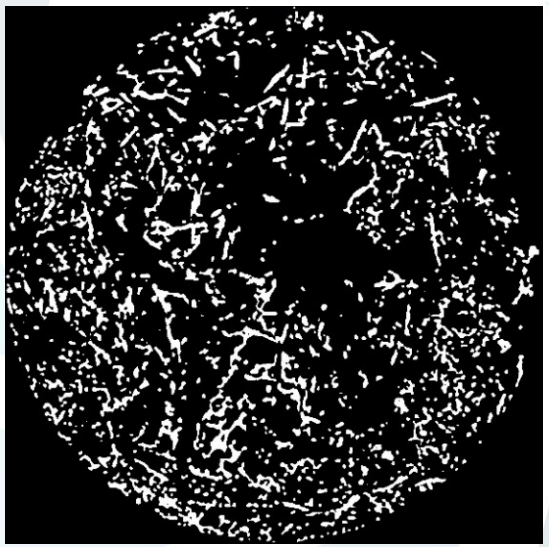


Acquisition

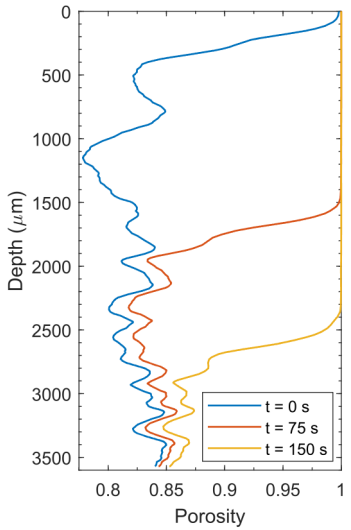
Raw 4D projection data



Reconstruction



Deep learning segmentation



Time-resolved carbon oxidation data

supercomputer

Porosity

Diffusion-Limited

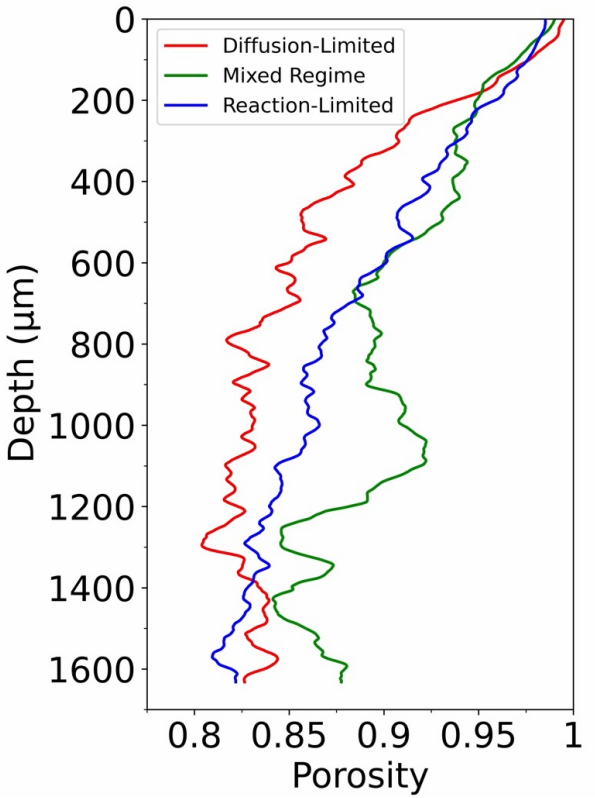
Power	18 A
Temp.	1320 K
Pressure	100.5 kPa

Mixed Regime

Power	15 A
Temp.	1060 K
Pressure	100.0 kPa

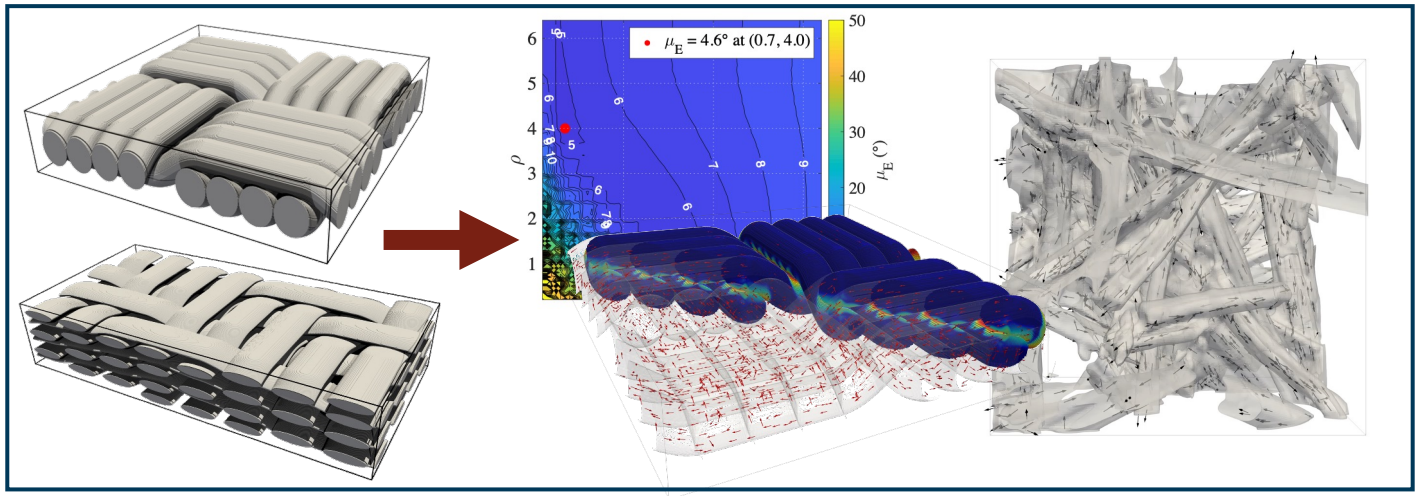
Reaction-Limited

Power	13 A
Temp.	945 K
Pressure	100.7 kPa

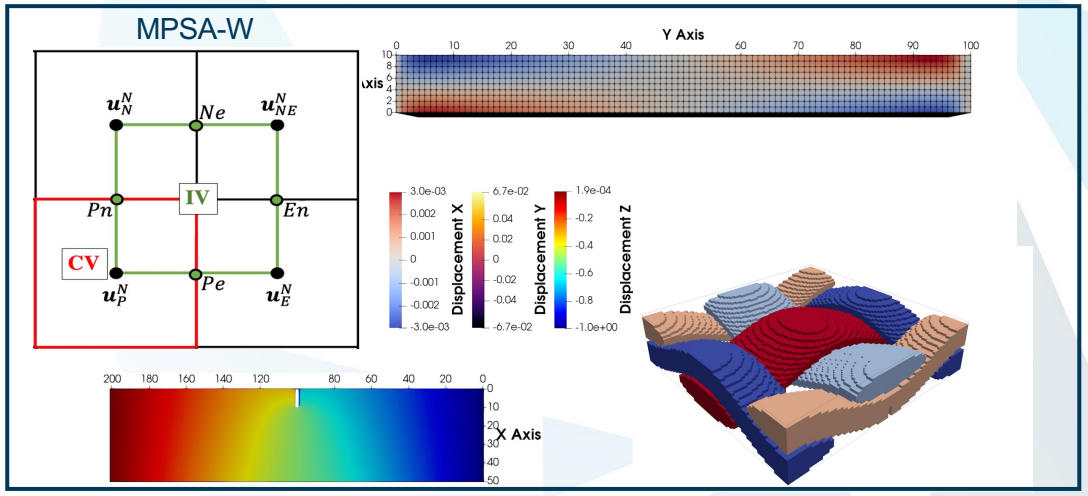


PuMA Property Computation

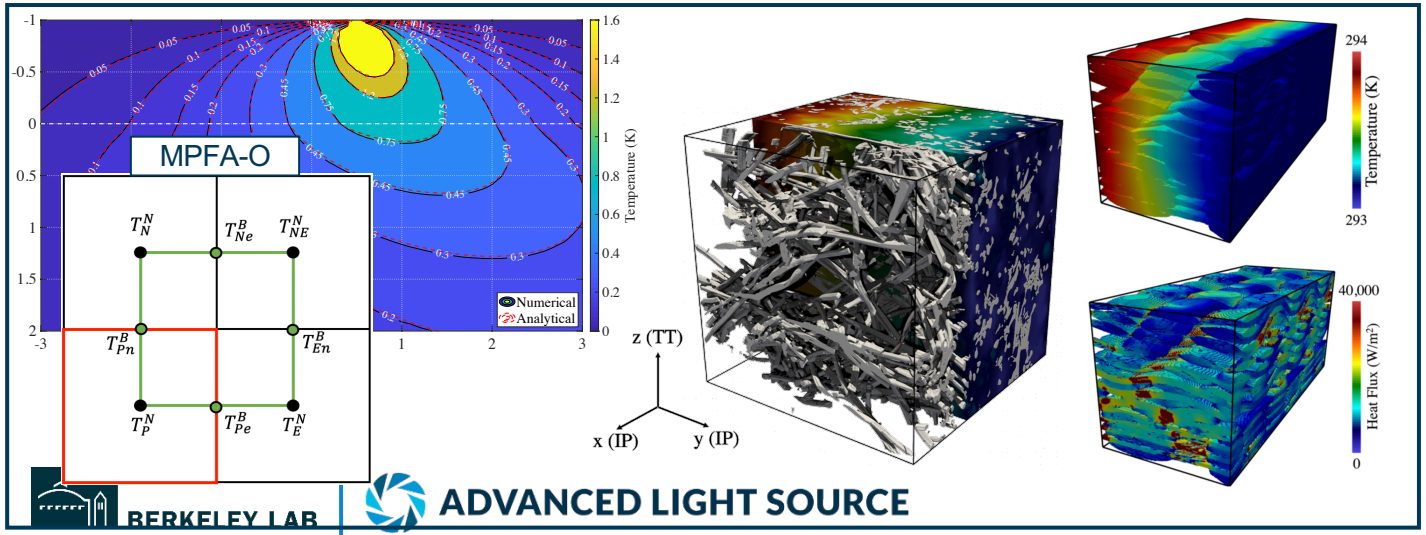
Material orientation. *Computational Materials Science* (2020)



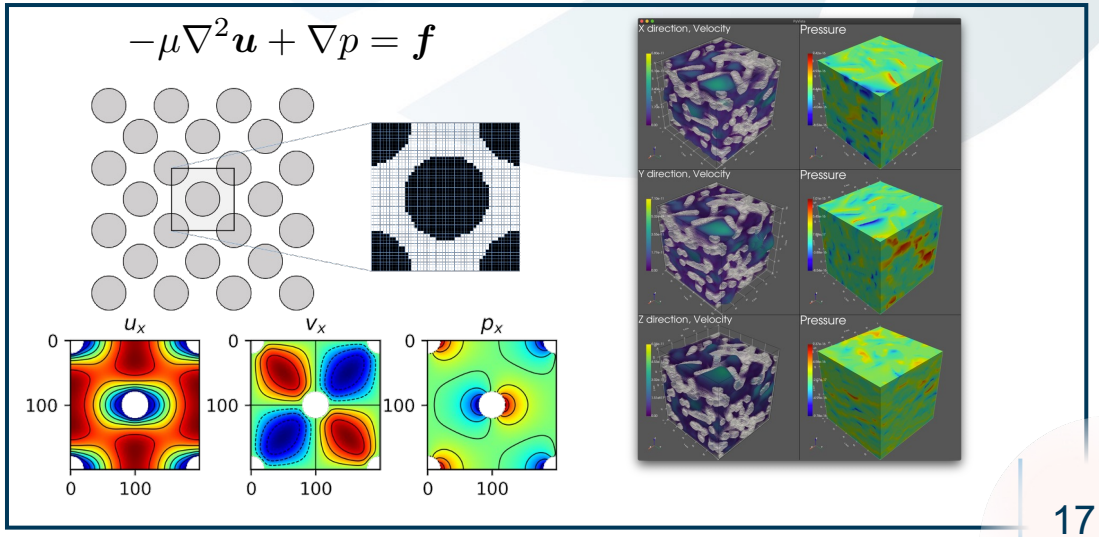
Effective elasticity. *AIAA SciTech Forum* (2022)



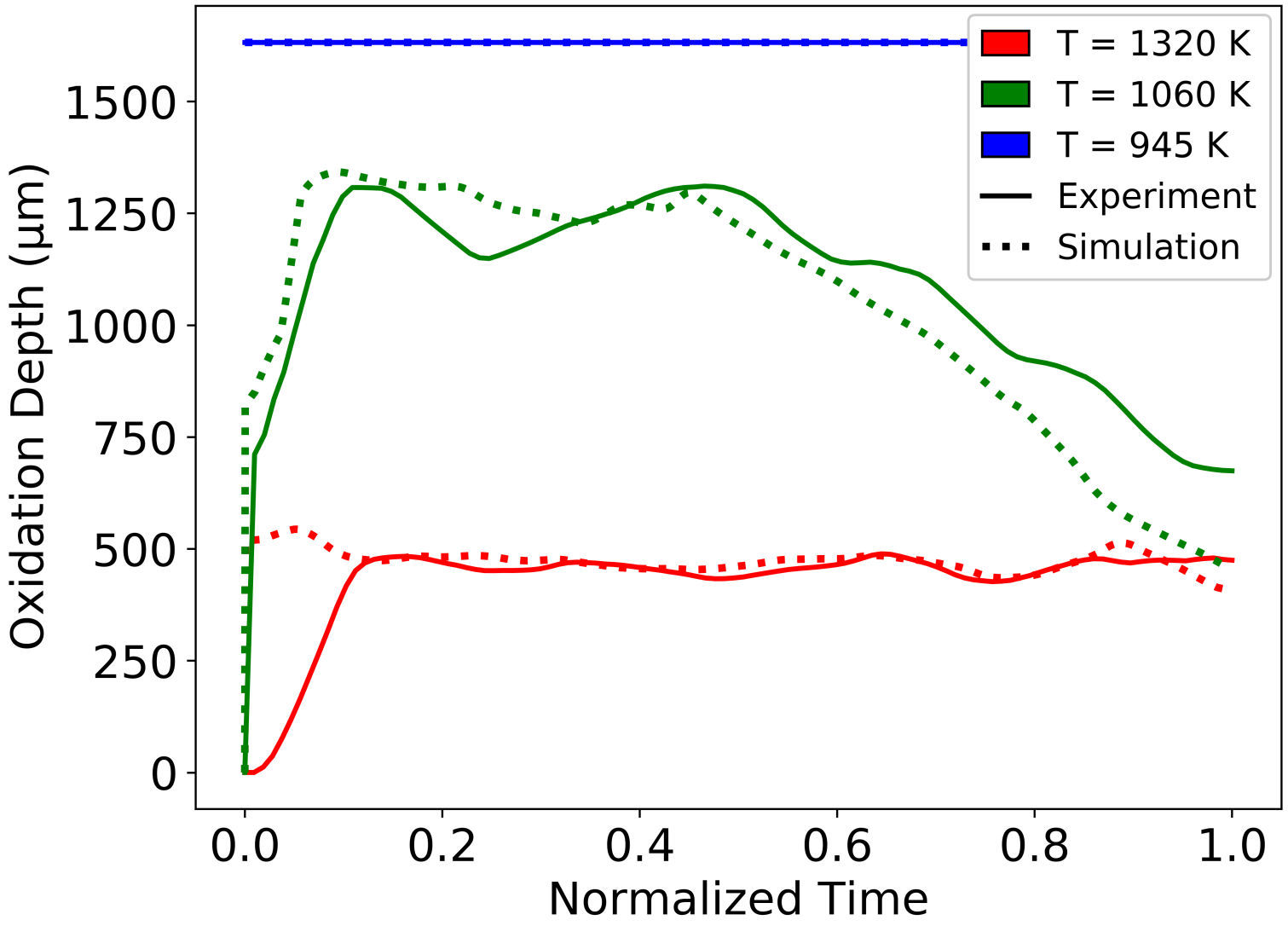
Effective conductivity. *Computational Materials Science* (2021)

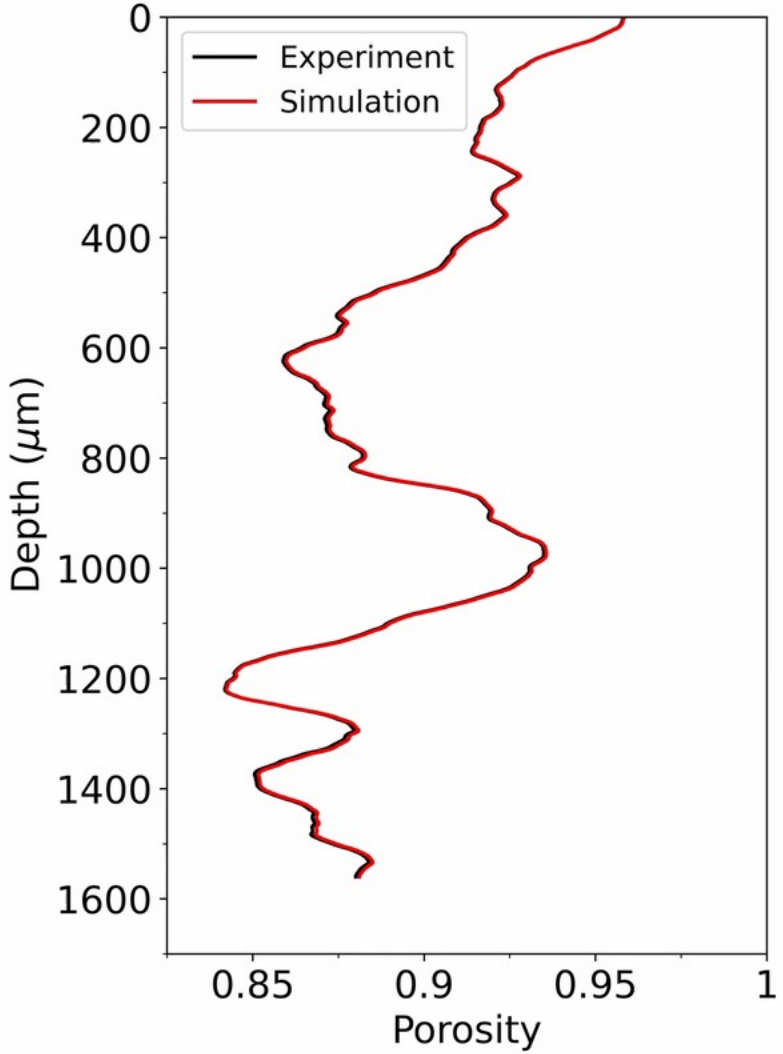


Effective permeability. *Computational Materials* Science (2023)



Simulation/Experiment Comparison





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!

Thanks! (this is a spider head)

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