SciCat

advance your data to advance your science

ALS Facility Updates

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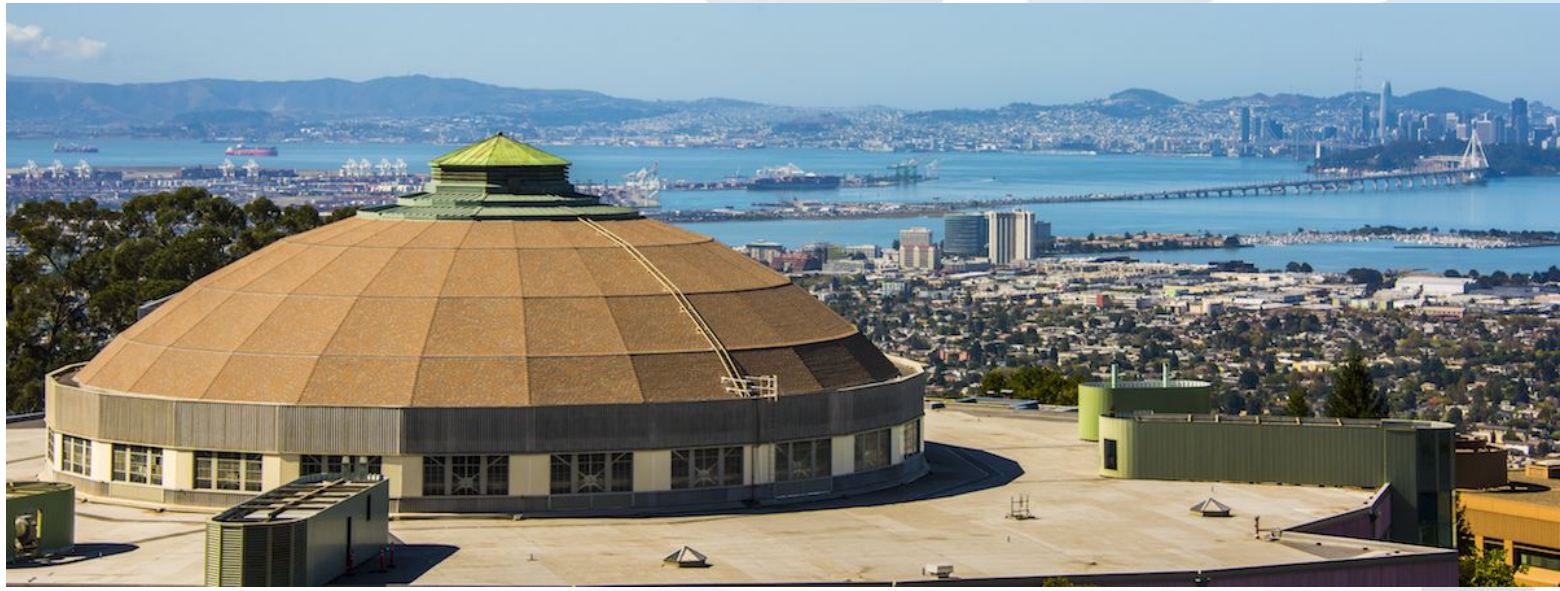
ALS Computing Group

ScicatCon June, 2025

ALS



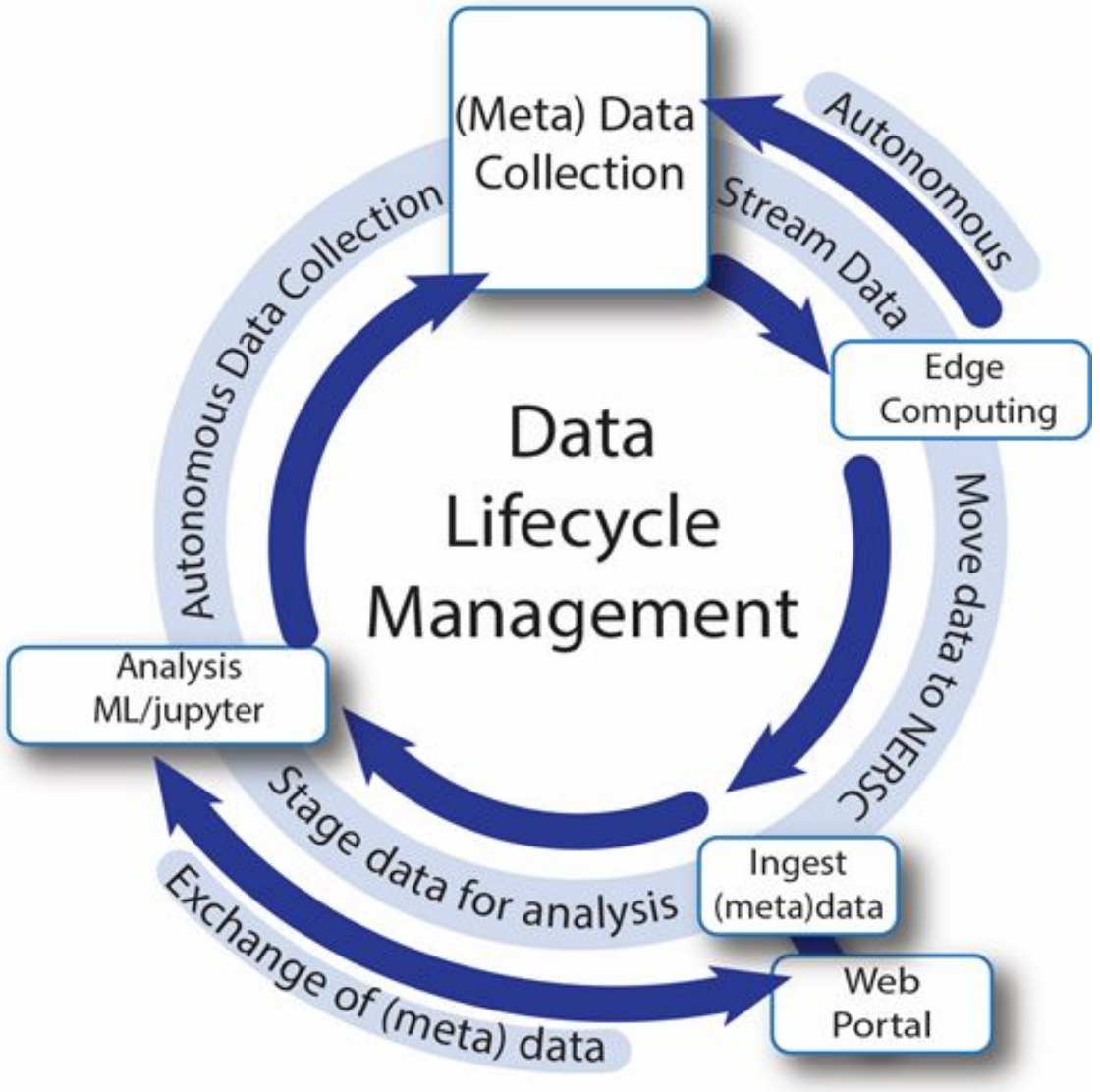
- 40 beamlines
- 2000 users per year
- 3rd generation
- 1 SciCat beamline
- Photon Sciences Computing Group
  - AI/ML
  - Workflows and Visualization
  - Data Infrastructure

ALS-U

- Dark in 2028
- ~ 2yr Darktime
- 1PB a day?

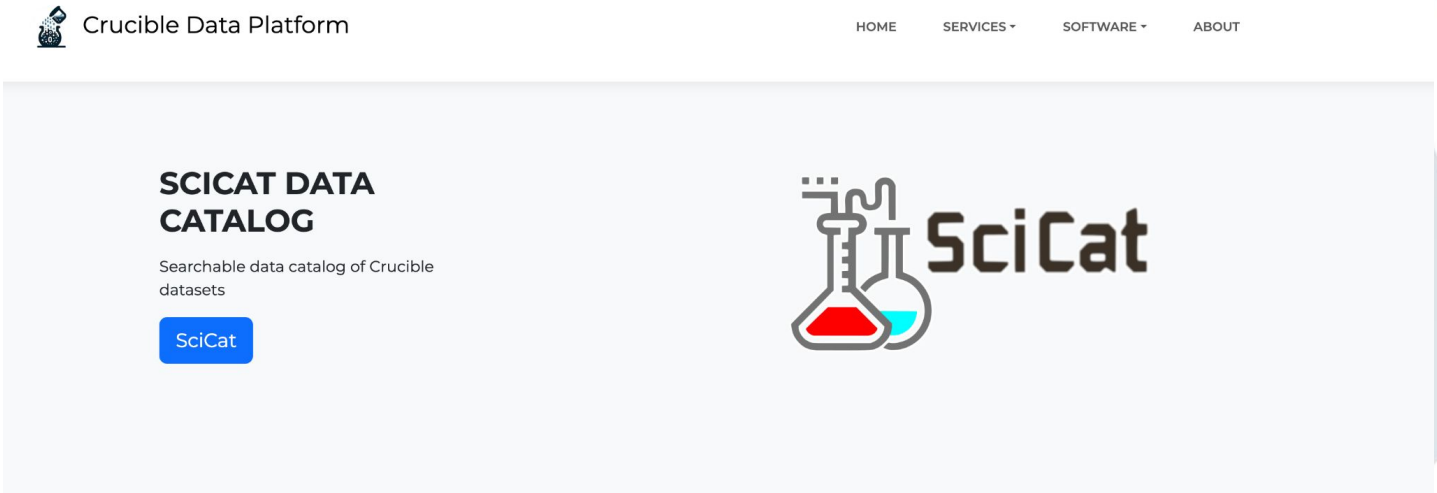
ALS Computing Program

The ALS computing program's mission is to **develop solutions for the mounting data challenge** and **help facilitate compute solutions for the Advanced Light Source**. The computing program **addresses the main challenges of the data lifecycle in close collaboration with the other four DOE light source facilities**.

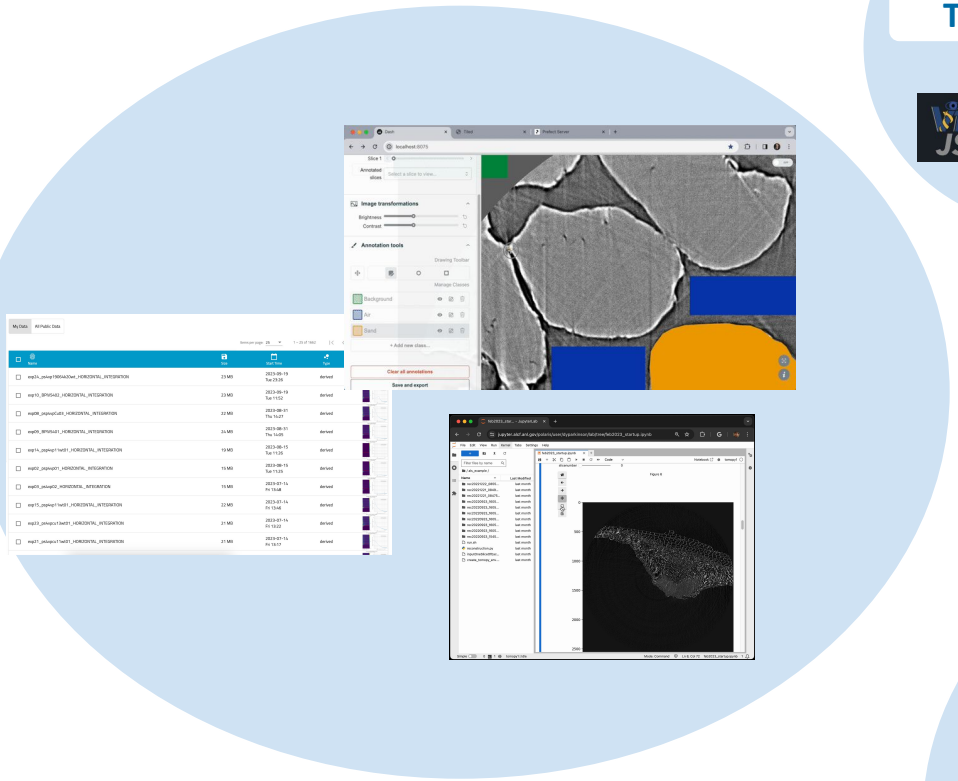


The Molecular Foundry

- Sibling facility
- Synthesis / NCEM
- 25% of ALS users are also TMF users
- Crucible Data Platform



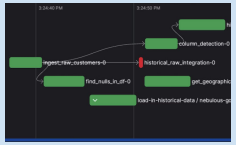
Data Orchestration



Tiled

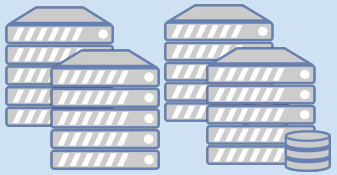
jupyter

plotly



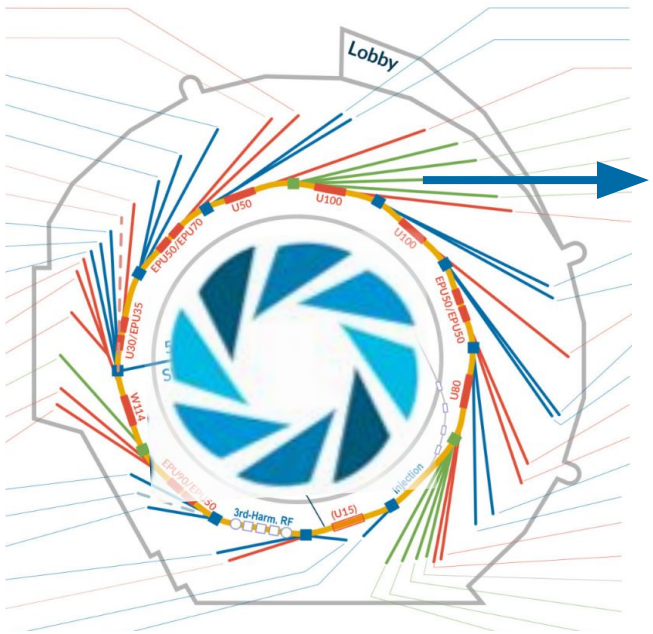
NERSC

beamline



Argonne NATIONAL LABORATORY

ASCR IRI



Measure

Raja S. and Wiebke K. prepare a sand sample and take a measurement.

globus

Computing Workflow

NERSC

Run full-scale reconstruction at NERSC on-demand, in near real-time.

- File-based
- Streaming

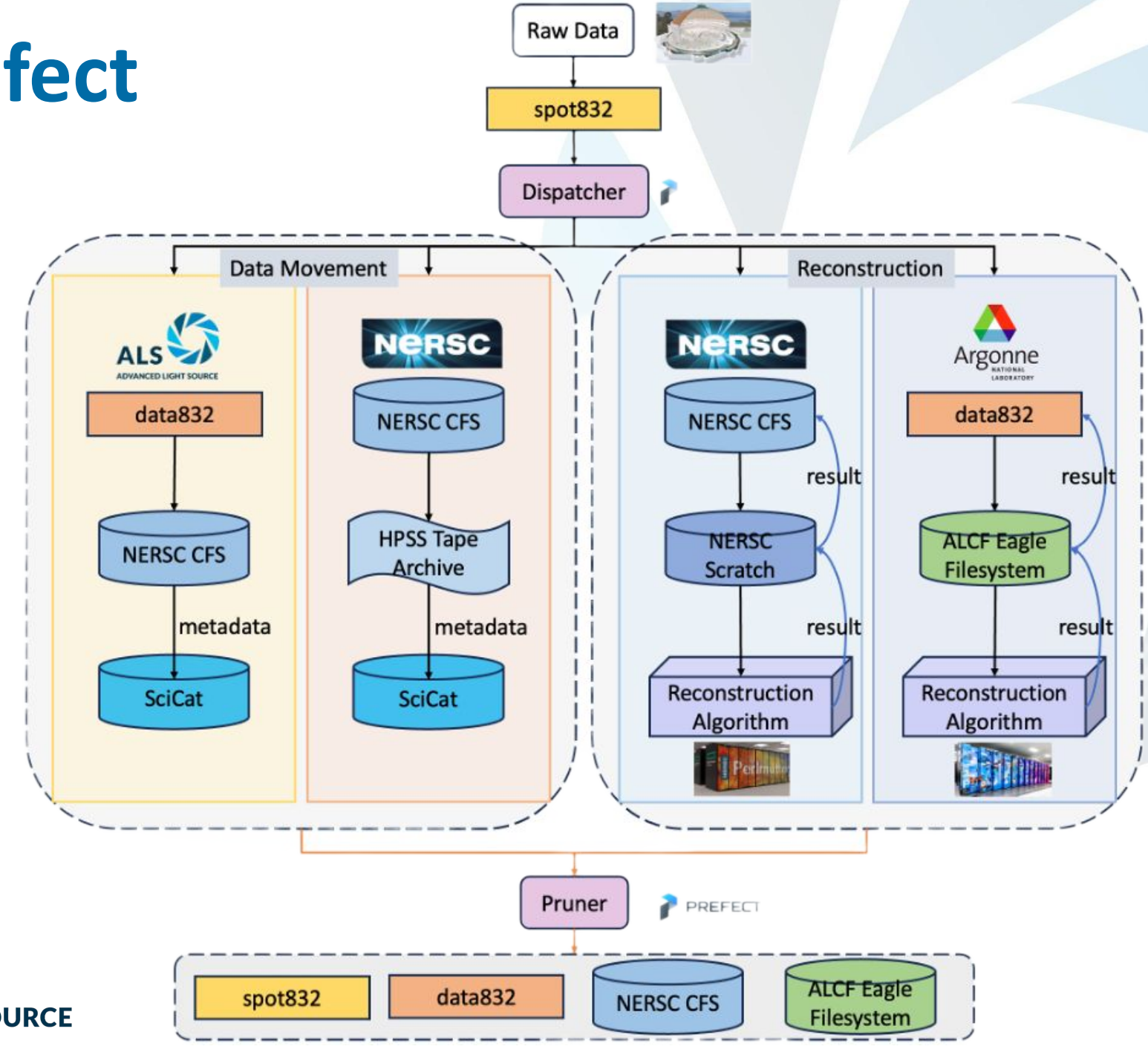
globus

Visualize Results

kitware jupyterhub

View processed scans with intuitive data-driven interactive web applications.

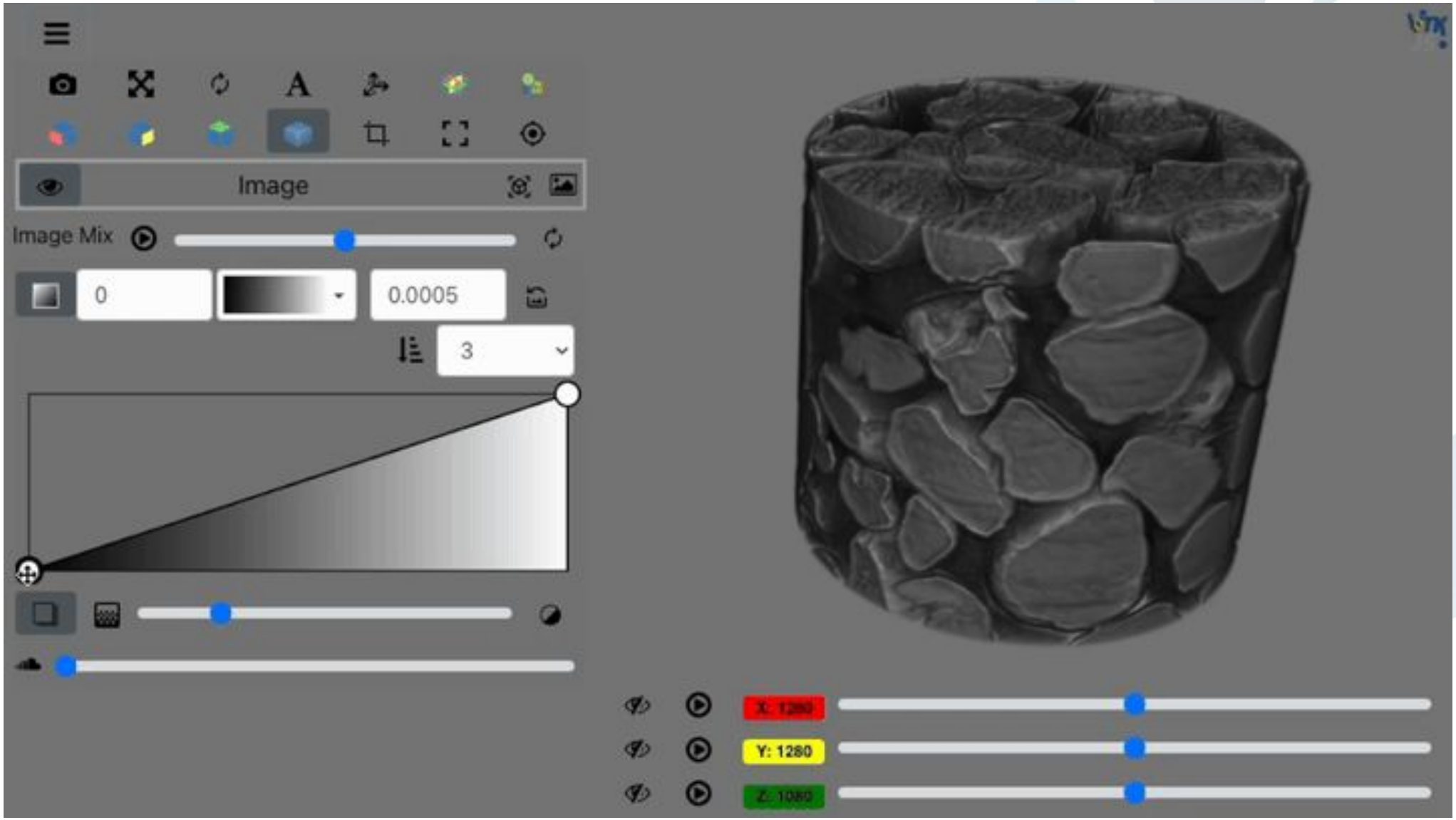
Tomography Prefect Workflow



Workflow Example

- Copy data to HPC
- Ingest metadata into **SciCat**
- Index data in and metadata into **Tiled**
- Run an automated reconstruction
- Create **multi-scale volume pyramid** for visualization
- AI enhanced segmentation
- Copy reconstruction to mid- and long-term storage
- Schedule pruning from intermediary file systems

Visualizations



DOE Data Mandate

- All Data taken at facilities must be open by the end of the 2025
- Will need some catalogs
- A lot of focus on AI

SciCat at ALS by the end of 2025

- 8.3.2 Tomography
- 7.0.1.2 Ptychography
- 7.3.3 Scattering
- 9.3.1 AP-XPS
- 11.0.1.2 AP-XPS/Scattering

Sample Metadata Tracker

radius

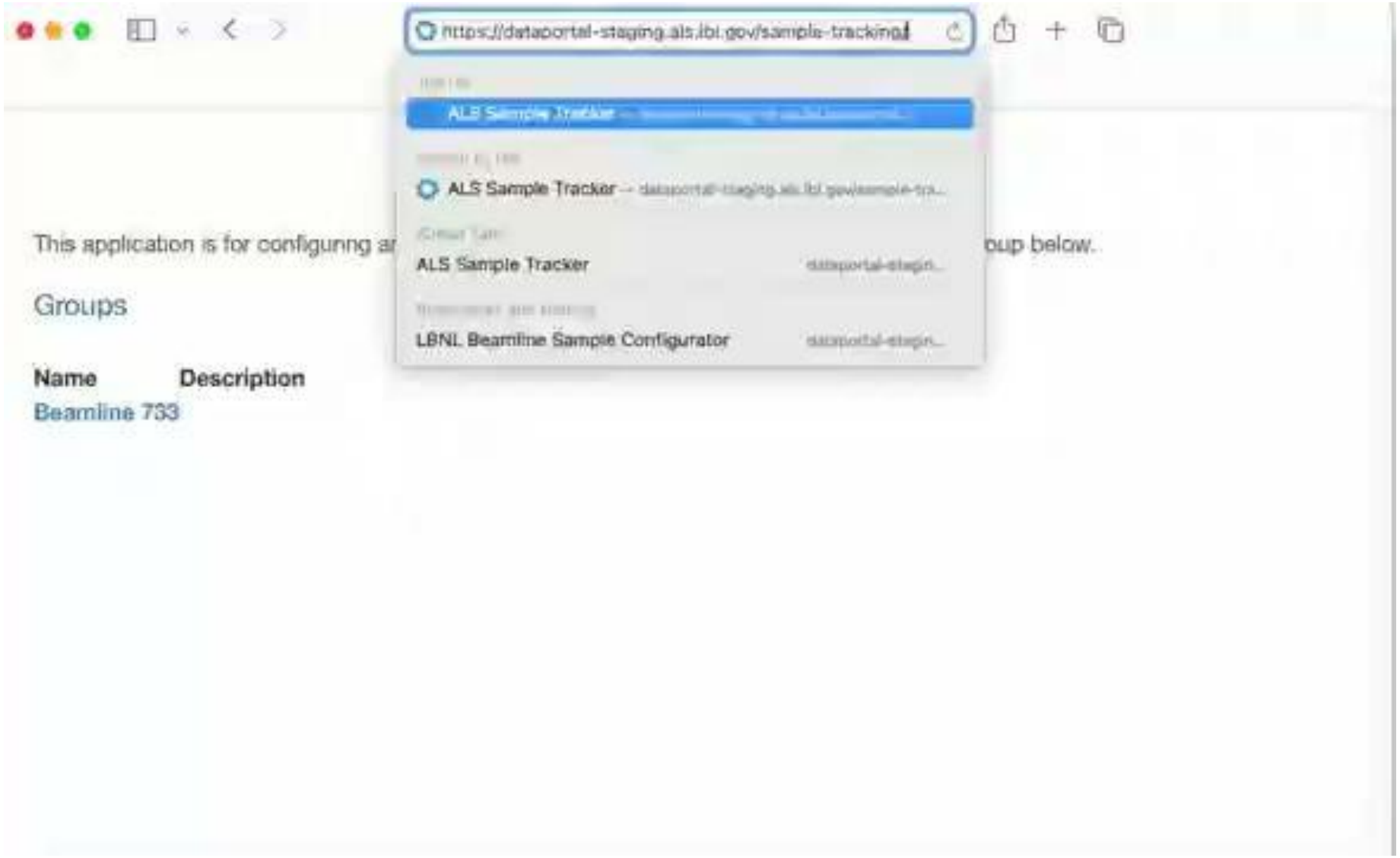
Rapid Deployment of Instrumentation for User Science

Photon Science small projects
Spring 2024

- Website where scientists can enter sample parameters in advance, before arriving at ALS.
- Each sample (and sample group) gets a unique identifier than can be used for all downstream operations.
- Identifier can be printed onto a label and attached to the samples.
- Robots can read the identifier and use it to fetch scan parameters automatically.
- We use SciCat to store data, and provide sample Python code to fetch it.

Sample Metadata Tracker

- Users log in with ORCiD
- They choose a proposal they have access to.
- Each beamline defines its own parameters.
- Interface validates data, and supports cut/paste and undo/redo.
- Labels print to a standard sheet.
- Persisted into SciCat Samples



Links Enhancement

- Backend Issue #689
- Link templates
- Metadata matching
- Add full links to the detail view
- Currently configuration file
  - selector-like matching based on dataset metadata
- Coordinate with Actions (selection, handlebars)
- Configuration management?

pyscicat

- Fixes for new backend login
- Still thinking about using python SDK

Short Term

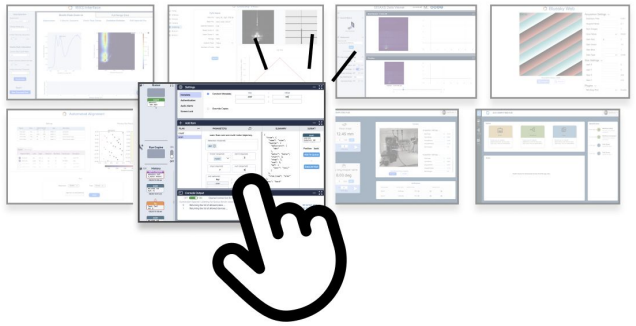
- More beamlines!
- Ingest Derived Data into SciCat
- Ontology / Schema definition and validation
- Integration with more data services
  - Tiled
  - Globus
  - GDrive (TMF Crucible)
- Visualizations
- Migrate deployment to cloud k8s (GKE)
- Implement Elastic

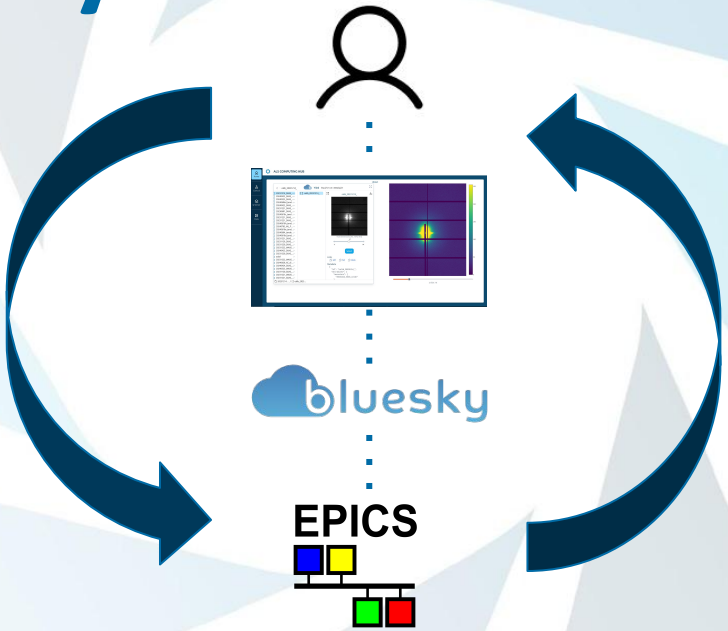
Further Out

- Data Access (globus, better application, tiled)
- Schemas
- Tagging/Labeling
- Multiple Search Engines
  - Elastic
  - LLMs
    - SciCat Agent
  - Federated Search

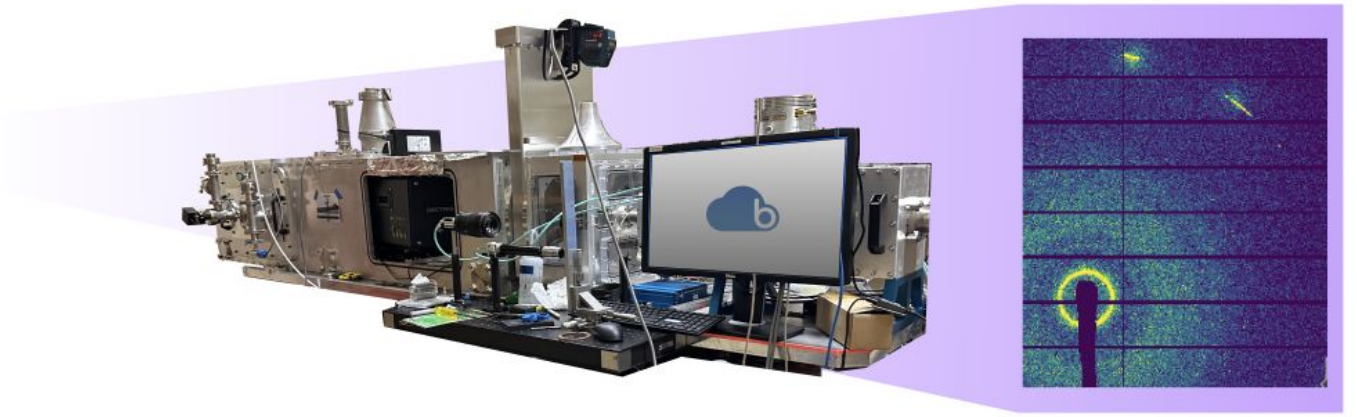
Web Based Beamline Controls/Analysis

Modularized React components from Finch UI library

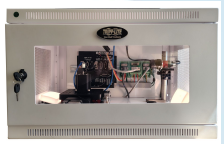


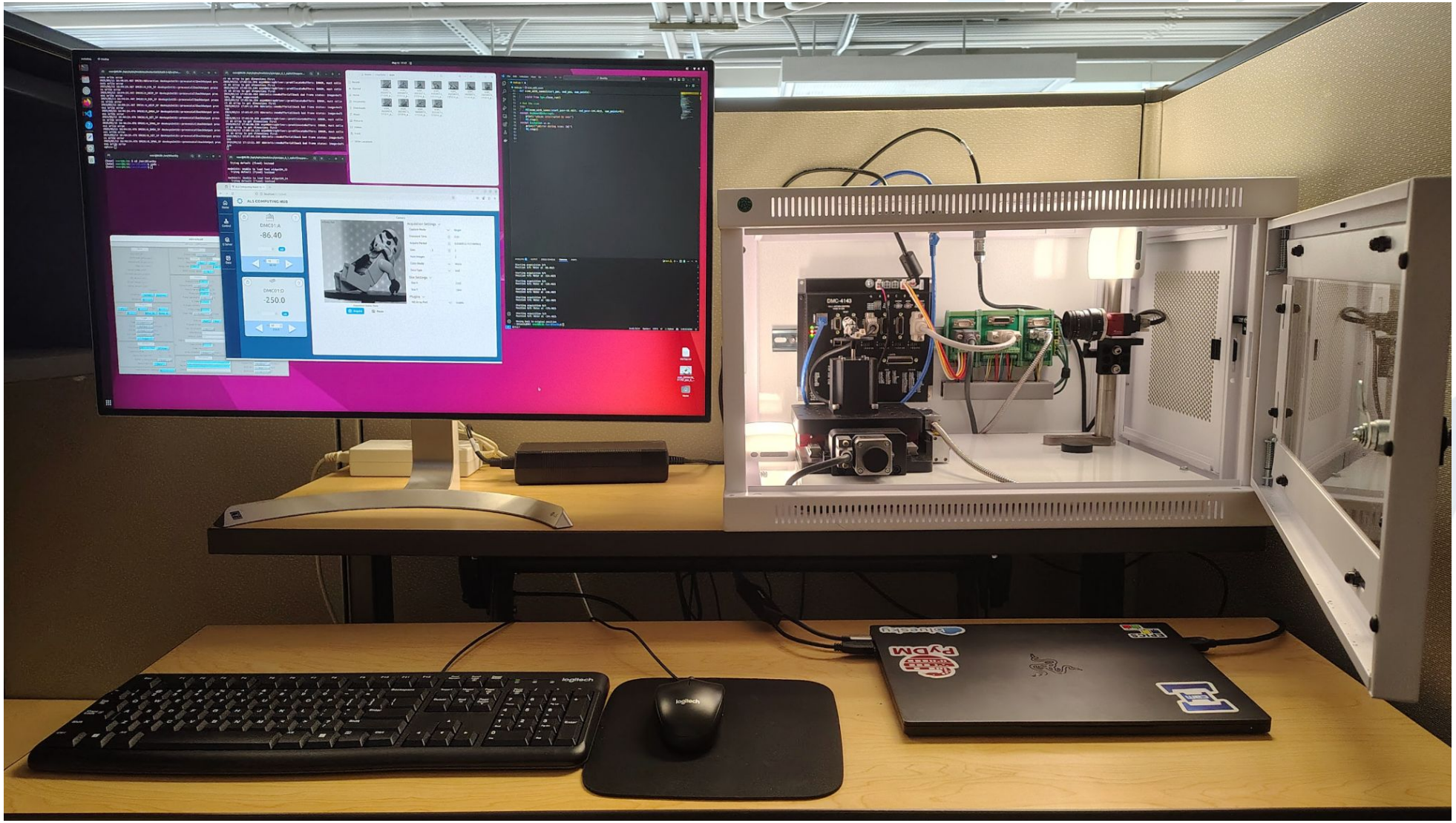


Experimental Orchestration and control with Bluesky



BOLT - Beamline Optics Learning Testbed





Thank You!

ALS

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Tracy Mattox
Mel Sibony
Andrea Jones
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Damon English
Kuldeep Chawla
Karen Fernsler

Scicat Team

All of you!

CRD

Harinarayan Krishnan

NERSC

Bjoern Enders
Spin Team