Data Opportunities

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BERKELEY LAB

U.S. DEPARTMENT OF ENERGY | Office of Science

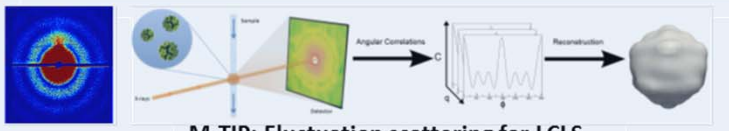
ALS ADVANCED LIGHT SOURCE

Data Management in Context

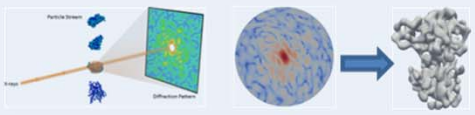
CAMERA: The Center for Advanced Mathematics for Energy Research Applications
ASCR-BES center building the mathematics for DOE's light sources

How does one efficiently frame and solve mathematically correct inverse problems to extract information from different acquisition modalities?

Goal: determine structure, function….

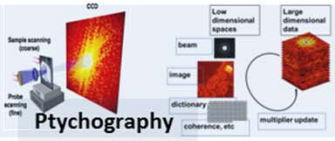


M-TIP: Fluctuation scattering for LCLS

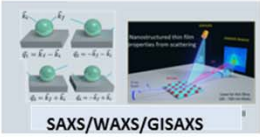


M-TIP: Single particle imaging for LCLS

TomoCAM: Fast GPU tomography for microCT



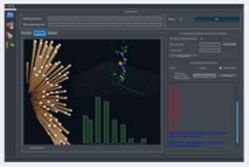
Ptychography



SAXS/WAXS/GISAXS

Once you get this information, how do you analyze it?

Goal: determine patterns, similarities, properties,..



FibriPy: Auto-detection of fibers and breaks in materials

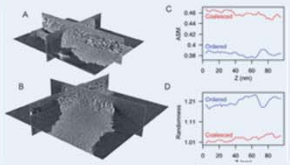
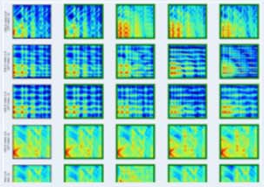
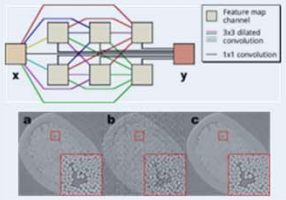


Image analysis for quality control during thin film manufacturing



PyCBIR: Deep learning for X-ray diffraction and materials.

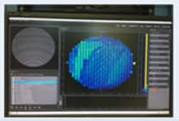


A new Mixed-Scale Dense Deep CNN for machine learning

What is the best way to use computing resources (embedded in detectors vs. local hardware/GPU vs. remote supercomputers) to quickly analyze results and guide new experiments?

Goal: Analyze/steer experiments as they happen

Nanosurveyor: Real-Time streaming for ptychography



On-the-fly Data Analysis for High-Throughput XRD

How you share algorithms, data, tools, and answers across the community?

Goal: Working together

Xi-Cam: Platform for Synchrotron Data

In use at 10 beamlines across ALS, SSRL, NSLS II, APS. Free

CAMERA+ALS+SSRL+NSLSII

Data Retention Policy

- ALS official policy
- Current practice

Official ALS Data Retention Policy

- We don't retain data
  - https://als.lbl.gov/data-management-and-transfer/

- Users of the ALS are responsible for meeting their data management obligations to their home institutions and granting agencies…Because the ALS does not have a facility-wide data archiving service or staff to manage the data, the user must generally make arrangements to copy data to their own storage systems or move the data to their home institutions.

Observed Practice at ALS

- Most BL scientists at ALS save a lot of data
- Outside of pilot project beamlines, retention methods are not pretty

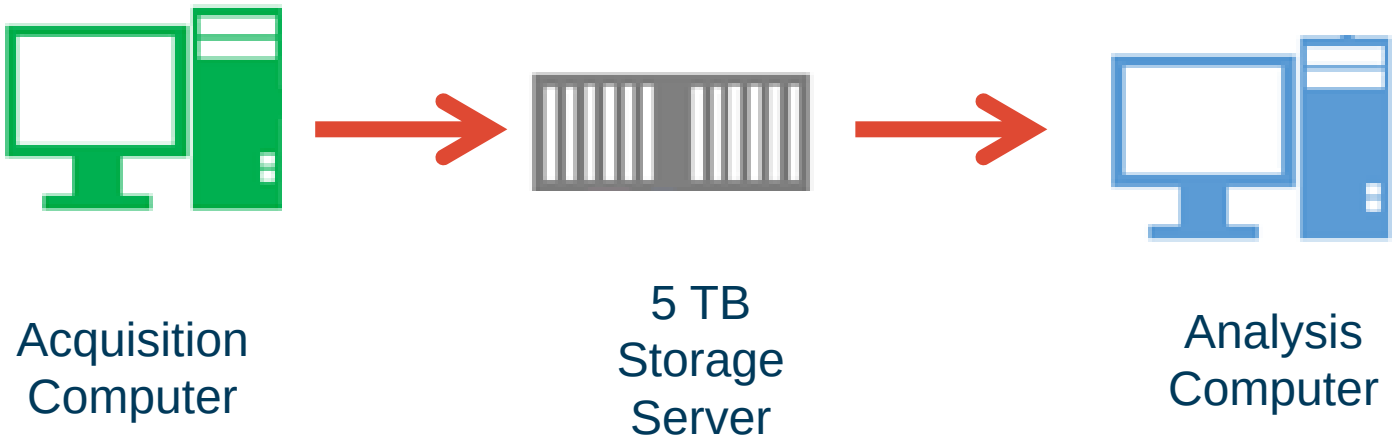
Photo taken in a Beamline Scientist's Office
5 October 2017

Experience With NERSC

- Why we started
- SPOT Suite
- Advantages and Challenges
- Super-facility

Beamline 8.3.2

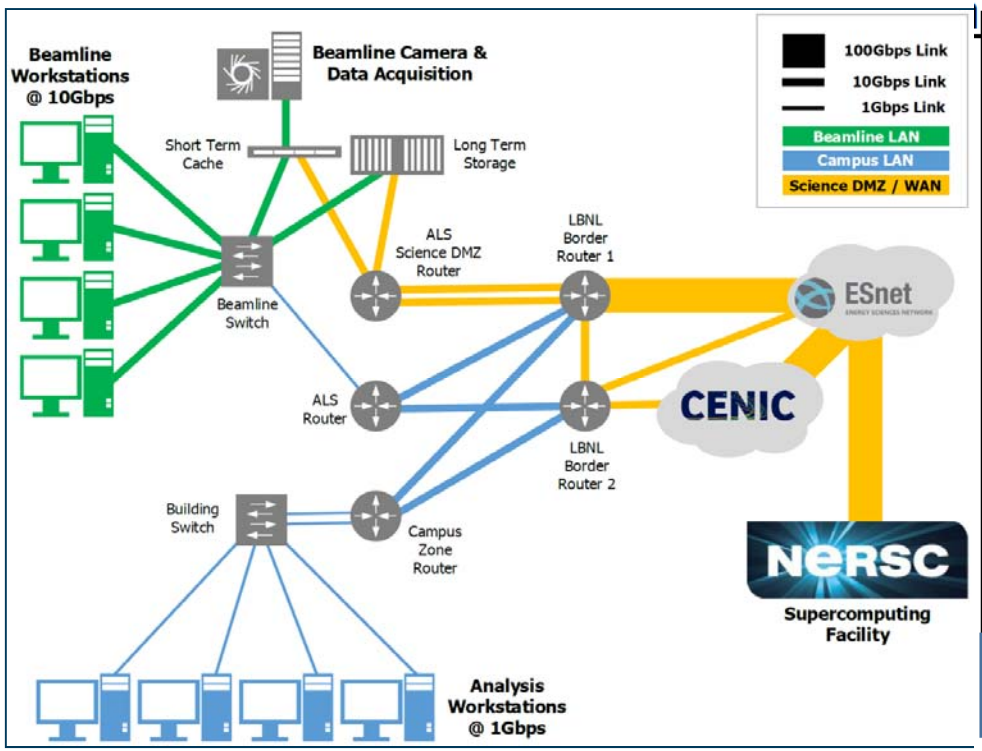
2010

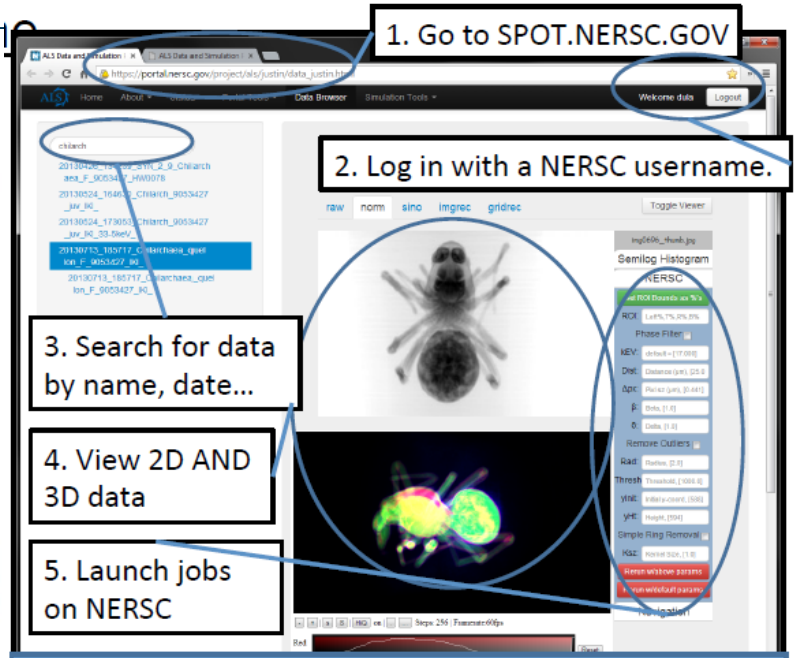


- After a new detector arrived in 2012, we could fill up our server in 1 day
- Something HAD to change

2012 LDRD: SPOT Suite

- Collaboration between ALS, LBNL Computing Division, ESnet, and NERSC

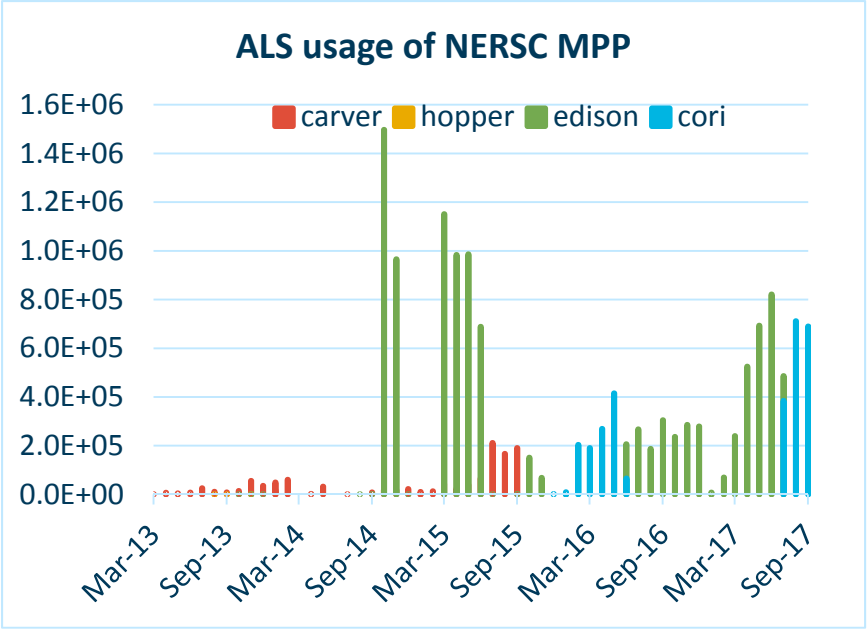


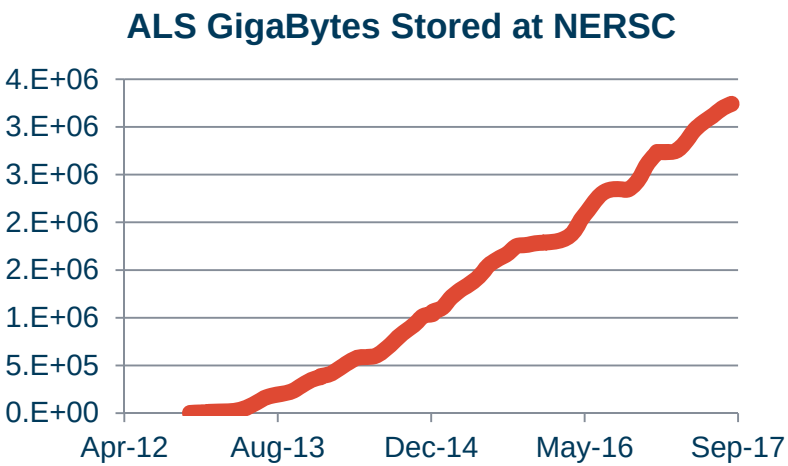


SPOT Suite transfers, processes, and presents data as it is collected, giving "real-time"

SPOT Suite: 3 Beamlines

- (as of June 2017)
- >365K data sets
- >3.0 PB on tape
- >5 million jobs
- ~250 beamline users



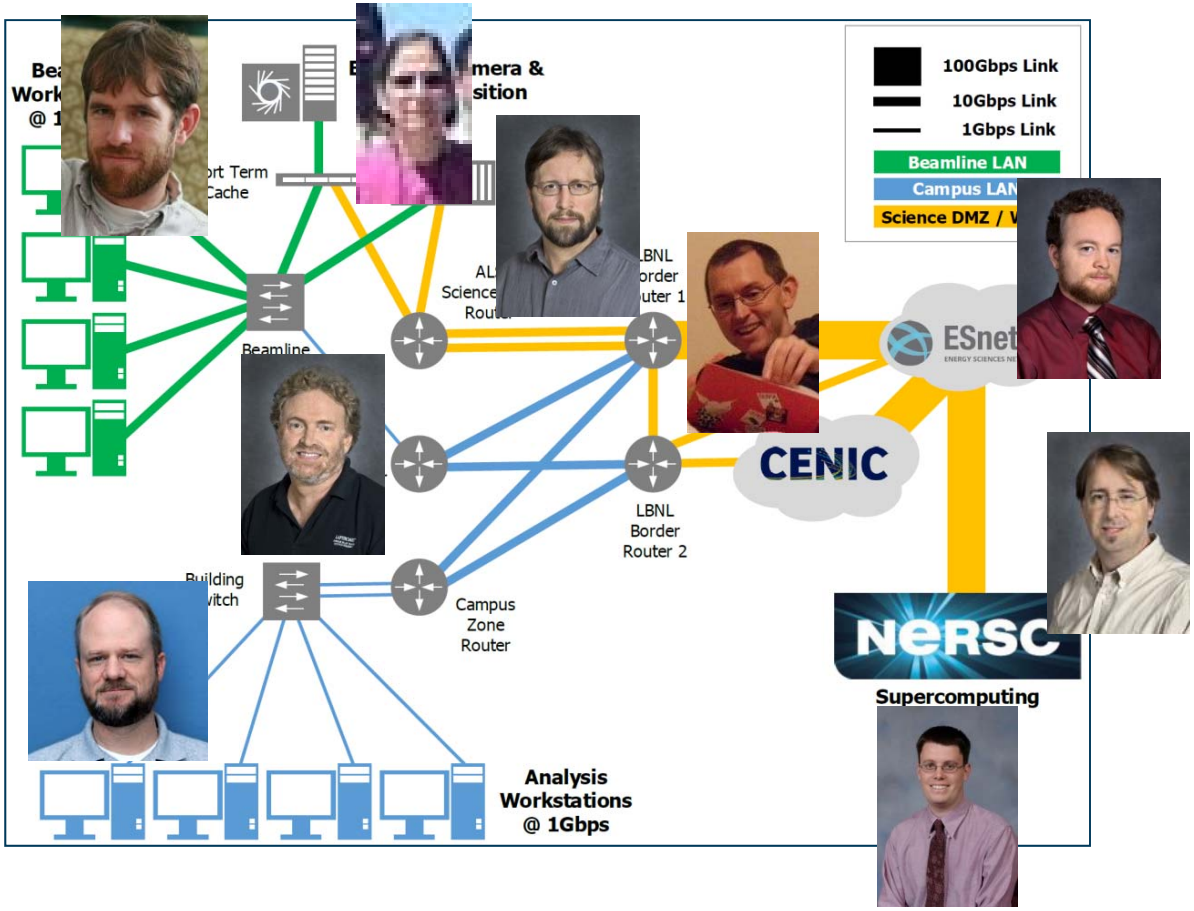


Advantages of SPOT Suite

- Searchable database
- Really fast network/data transfer
- Large amounts of storage
  - Automated purging of local storage after tape archive
- Users access data from NERSC directly
- Launching jobs on the supercomputer, with enormous compute resources
  - ALS 2017 allocation: 40 million hours

Challenge 1: Single-point failures

When a user calls me to say “I can’t see my data,” where do we find the problem, and who can solve it? (The beamline scientist is not in control)



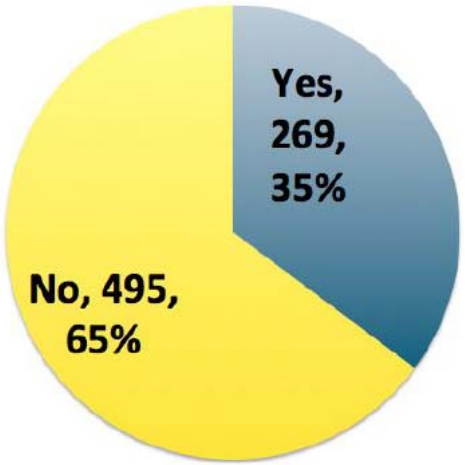
Other Challenges

- Potential for radical changes in architecture every few years as NERSC pursues cutting edge capabilities
- NERSC is not guaranteeing 24/7 uptime (spend resources on higher performance rather than robustness)
  - And how much 24/7 support is NERSC willing to give for facility needs
- How much computing can be reserved or is available for real-time queues
- How much storage space is made available
- No federated identity: at ALS BL832, users get separate accounts for alshub, beamline, globus, and NERSC

NERSC "Super-facility Initiative"

- NERSC is aware that it remains a challenge to use them as part of a super-facility, but they have plans to make it easier as more of their users want those capabilities
  - 2017 NERSC Survey: Does your project in some way work with experimental and observational data?

I was recently asked by somebody who answered no: "What the #%$! are you running on a supercomputer for?"



764 projects

My recommendations:

- Users experience one simple interface for data management and analysis/viz
  - Xi-CAM is a step in this direction
- Design robust data management systems with few single point failures
- Use modular components, many of which could be common to all light sources
- Leverage NERSC storage, compute
- Change retention policy: volunteer Light Sources to do this (and get resources to deliver)

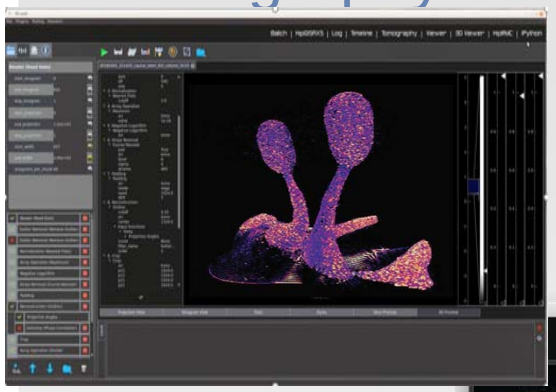
Extra Slides

- Data Flows comparison
- Xi-CAM (multi-mode and facility)
- Data Demo
- ALS Approach

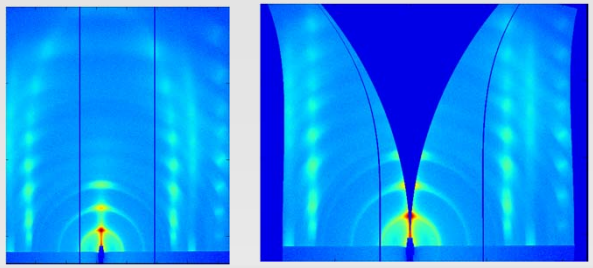
Xi-CAM

A. Hexemer[1], R. Pandolfi[1], D. Kumar[1], L.A. Pellouchoud[2] , C. Tassone[2], H. Parks[1], D. Parkinson[1], G. Freychet[1], Z. Jiang[3], A. Mehta[2], H. Krishnan[1], K. Yaeger[4], M. Fukuto[4], T. Caswell[4], F. Ren[2], D. Allan[4], S. Campbell[4], D. Gursoy[3], F. DeCarlo[3], **J. Sethian**[1]

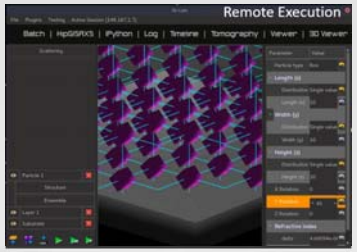
Tomography



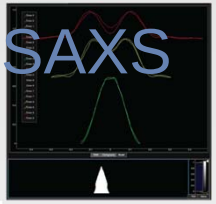
GPU accelerated corrections

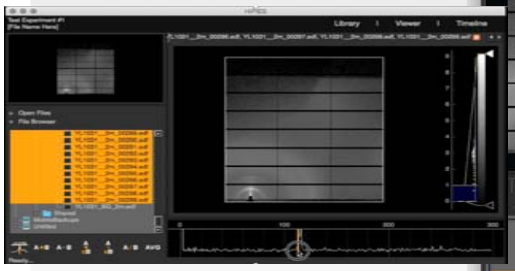


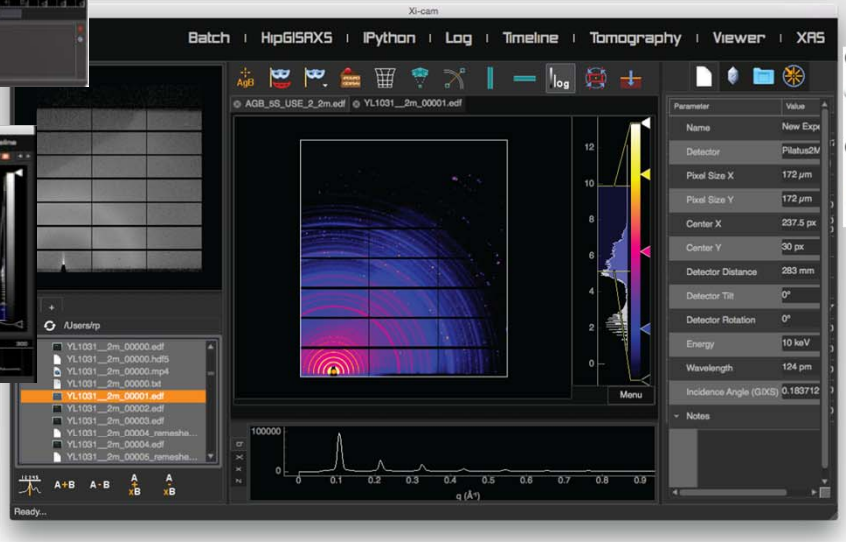
HIPGISAXS



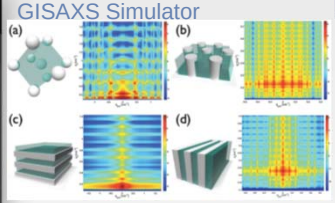
CD-SAXS

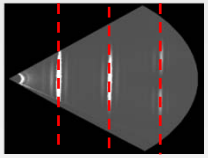




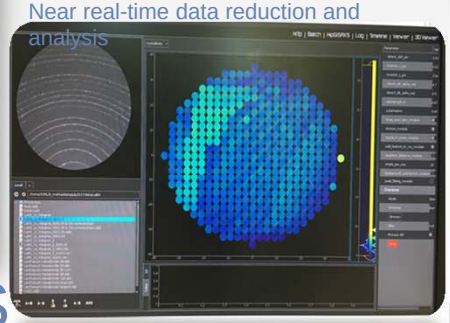


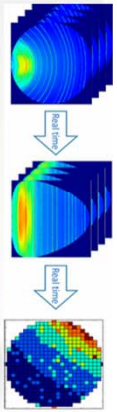
GISAXS Simulator



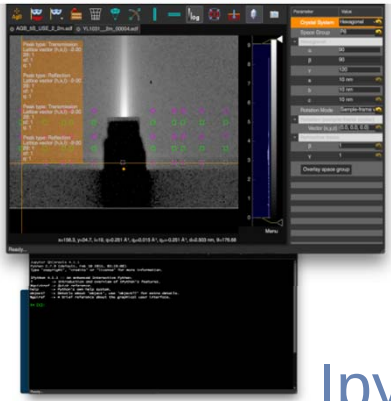


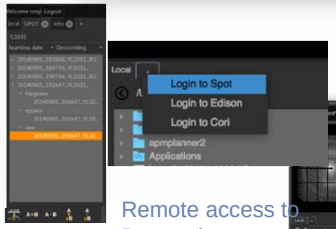
Near real-time data reduction and analysis





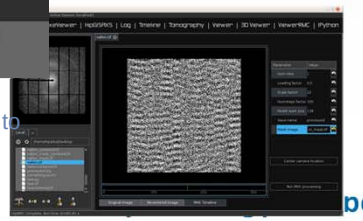
GIWAXS simulator



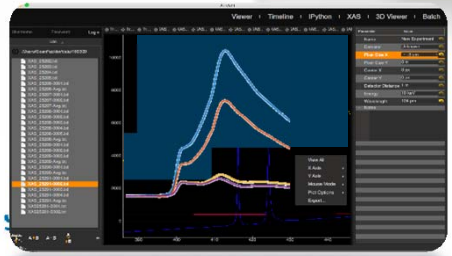


Remote access to Data using GLOBUS

revMC

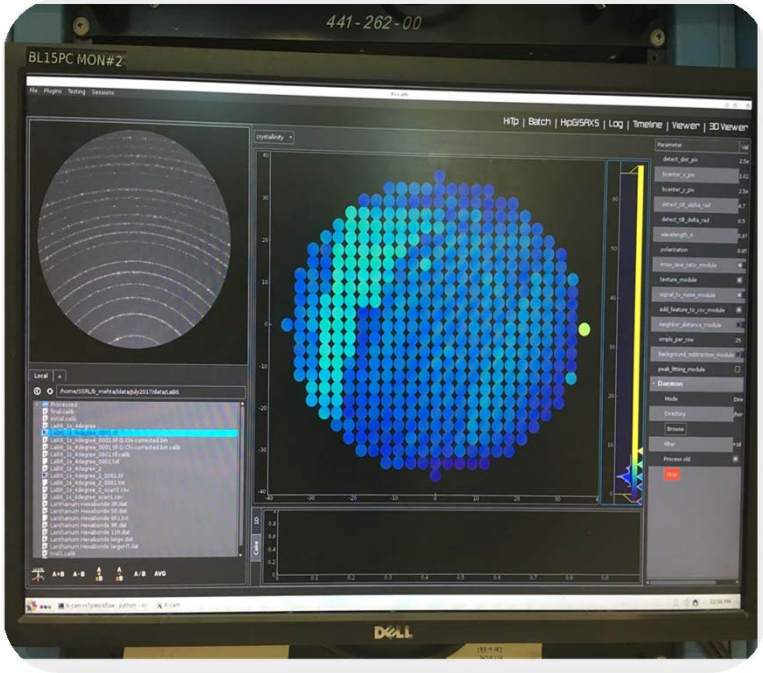


NEXAFS

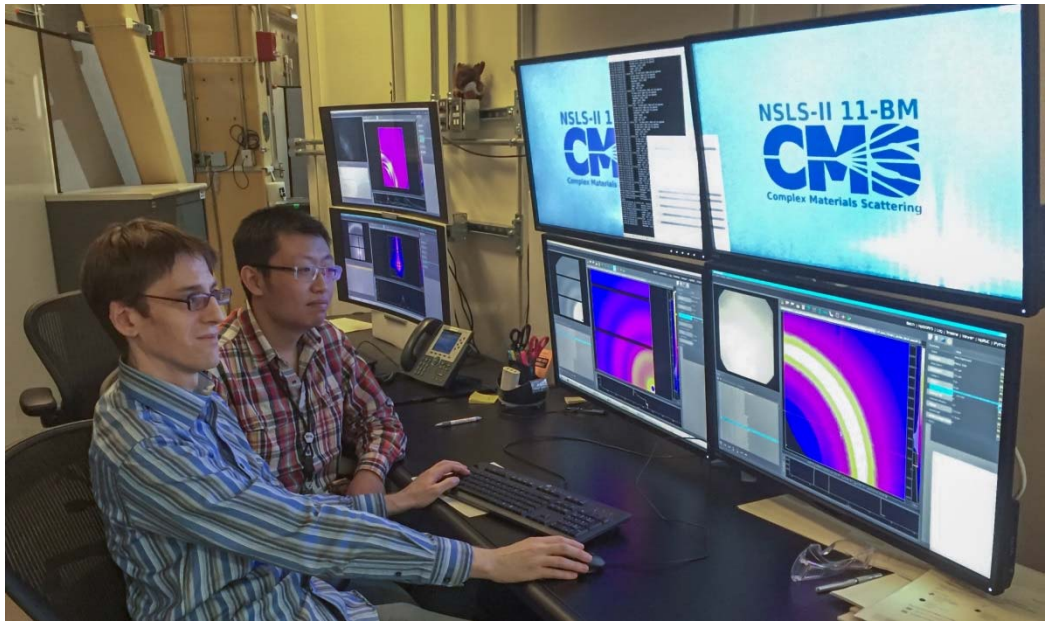


Ipython

Near real-time data reduction, analysis and feedback

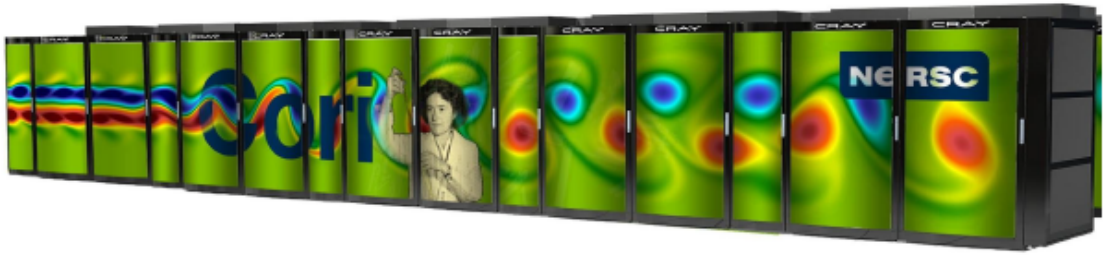


Xi-CAM running in real-time analysis mode at SSRL



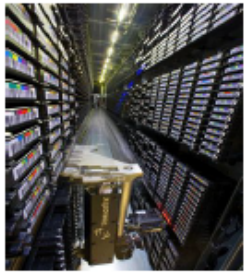
Xi-CAM running at the NSLS II CMS beamline in live analysis mode

2017 NERSC Resources at a Glance



Edison: ~3PFs, 8PB disk

NERSC Global Filesystem: ~12PB



HPSS Archive: ~100 PBs

Cori: 30PFs, 30PB disk
> 9000 Intel KNL nodes
> 2000 Intel Haswell nodes 'data partition'
Burst Buffer - 1.5TB/sec
Robust application readiness effort

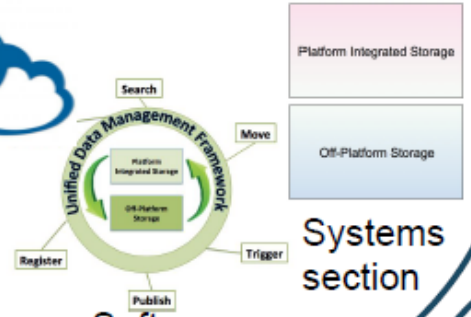
Superfacility API Functionality

Job management: submission, monitoring, retries

slurm workload manager

newt

Data Movement: Between layers, across facilities



Systems section

Software section

Reservations: HPC, Storage, BW

SDN

slurm workload manager

Publish and Share Data

OpenMSI

ALS

Manage Identities

Ø

Superfacility API: 2020

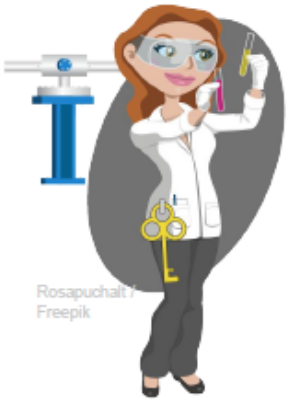
User at remote site: adjust and recalibrate

Submit data analysis jobs

Extract results

Publish and share data

Users

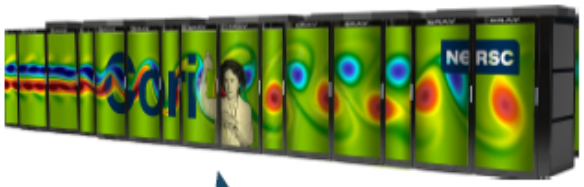


Strong engagement to make a useful UI (Section 4)

Superfacility API

Job management

Query system health



DBs

Science Gateways

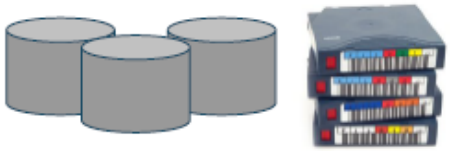
Spin

Workflow Manage-ment

Manage identities

Reservations (storage, CPU, BW)

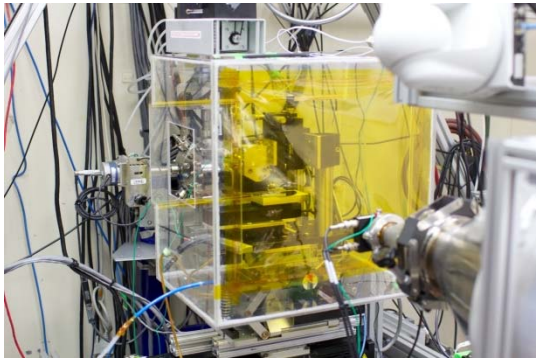
Create and control services with Spin



Data movement and sharing

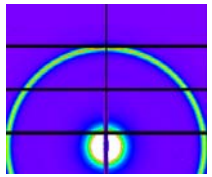
SAXS-WAXS Data Demo

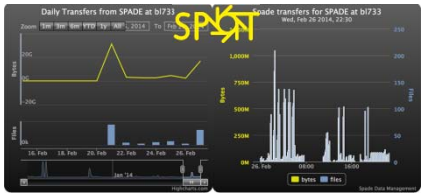
Collect data at 7.3.3



Transfer to NERSC

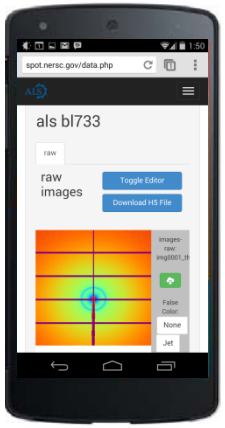
Pre-Process





Launch job at TITAN

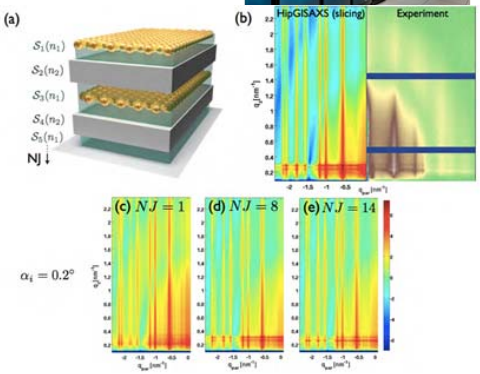
Launch job at NERSC



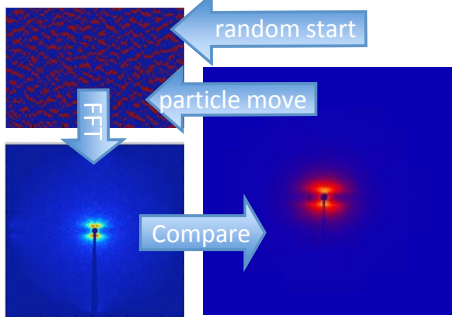
SPOT Manages Data Transfer, Workflow, and Presentation

View Results Anywhere

HipGISAXS (CAMERA)

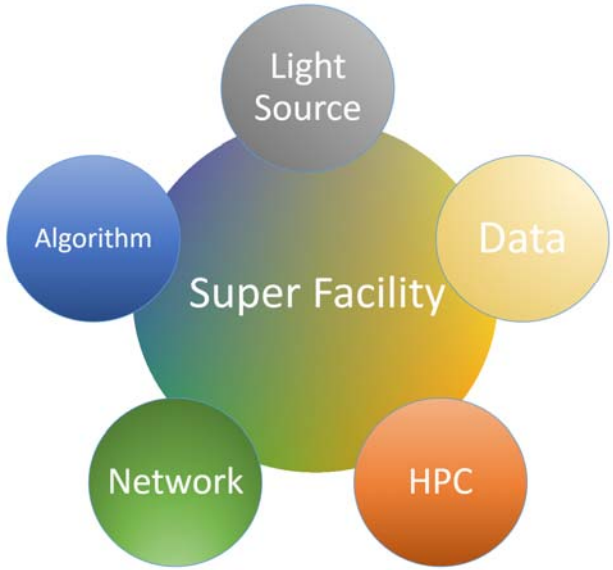


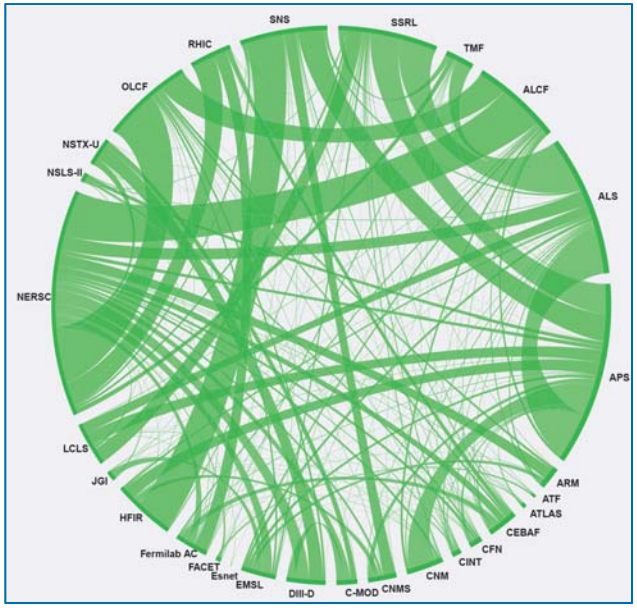
HipRMC



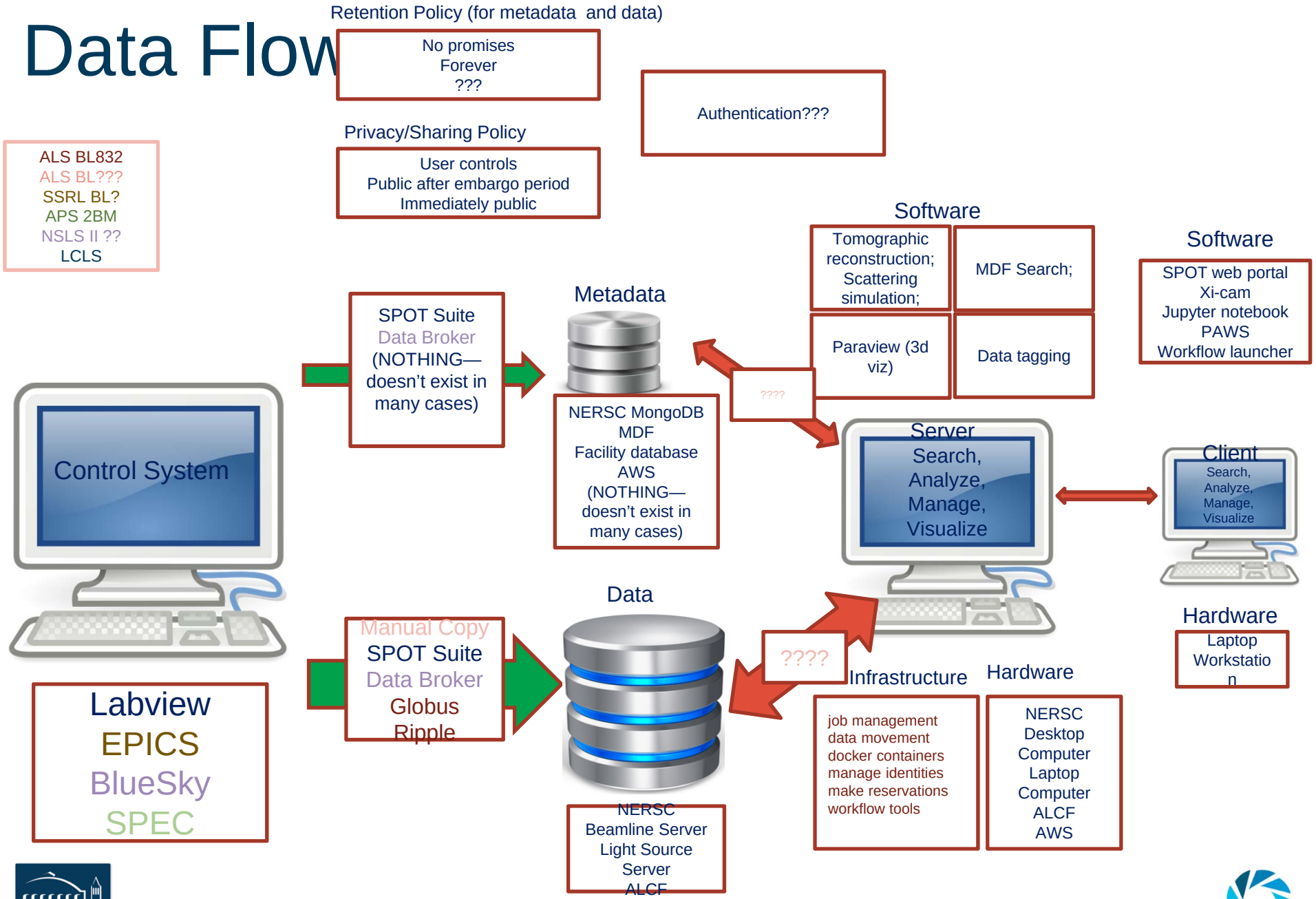
The ALS Approach

- Exploring cost-effective ways to contribute throughout the research cycle
  - Often different for each beamline-expertise must be embedded at each
- Collaborate
  - with computing
    - Many individual collaborations
    - CAMERA
    - SPOT
    - NERSC
    - ESNet
  - with other facilities





Data Flow



Acquire Store Compute Interact