Synchrotrons and Supercomputers

Dula Parkinson, Advanced Light Source

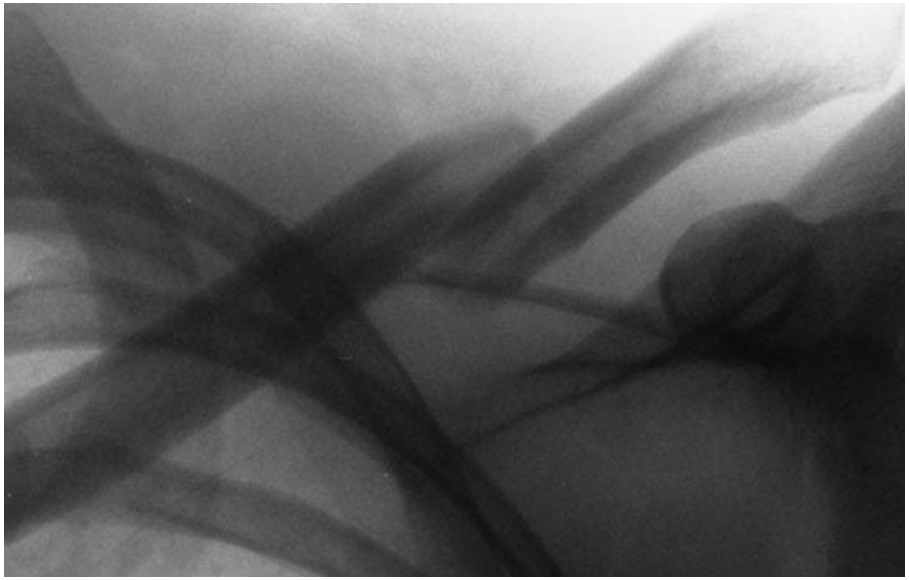
March 7, 2018

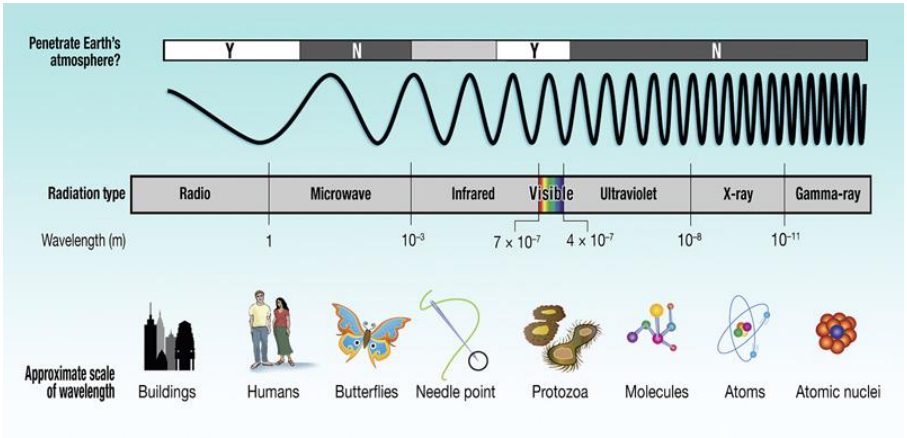
BERKELEY LAB

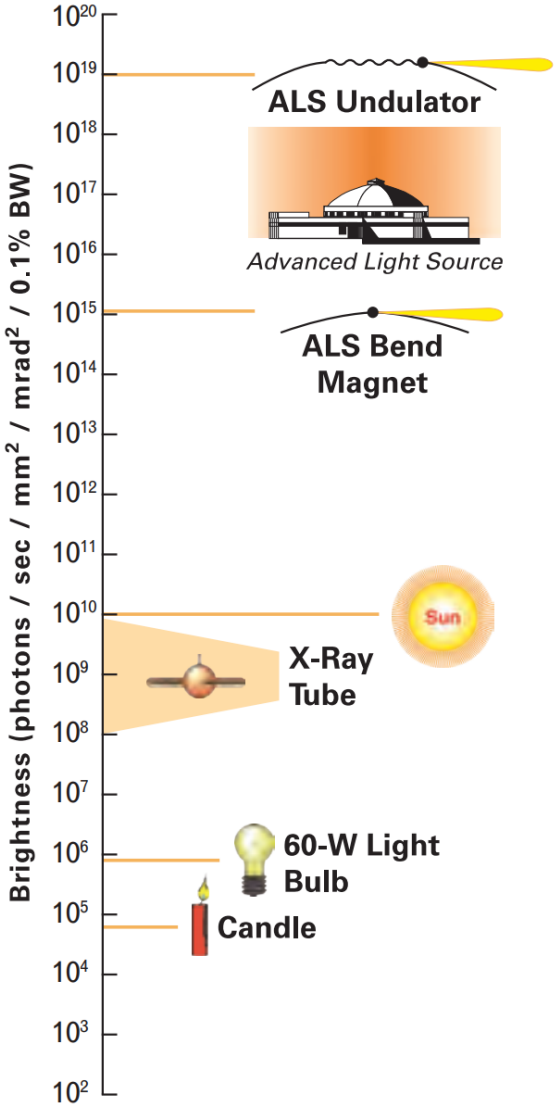
U.S. DEPARTMENT OF ENERGY | Office of Science

ALS ADVANCED LIGHT SOURCE

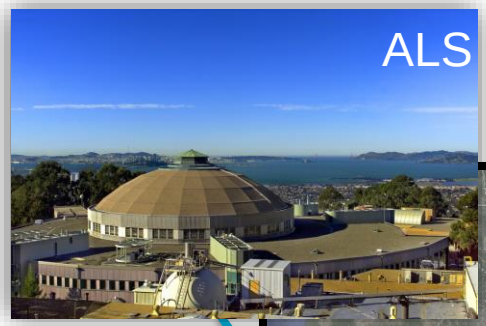
X-rays have unique capabilities
Light sources produce bright beams

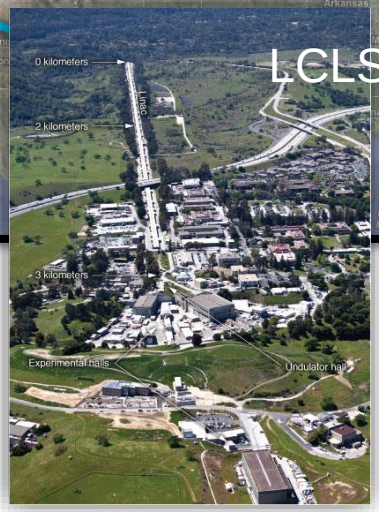






Department of Energy Light Sources





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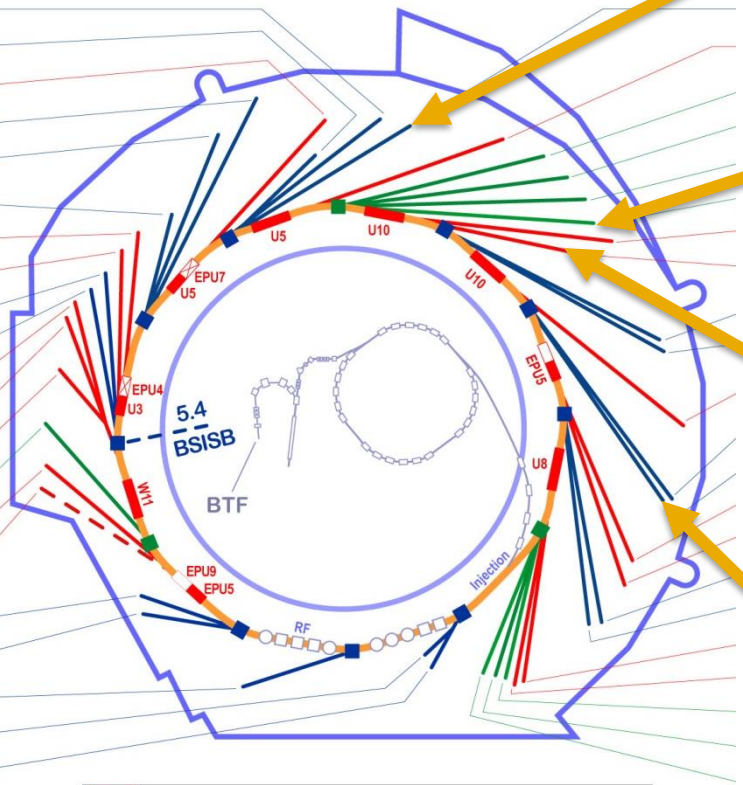
("light" = X-rays, mostly) ALS

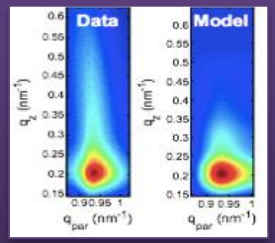
“Beamlines”



KEY	Operational	Comissioning
Insertion Device Beamlines	Bend Magnet Beamlines	Superbend Beamlines

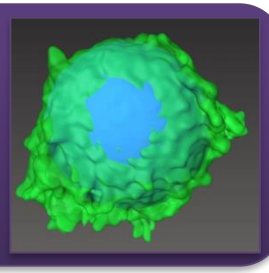
Reciprocal Space
(Scattering)

HipGISAXS/HipMC
parallel Scattering



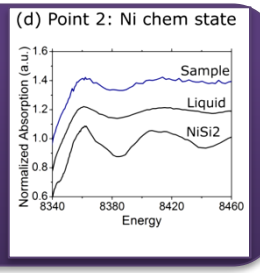
Real Space
(Tomography)

Arec3d, QuantCT,
CrunchFlow



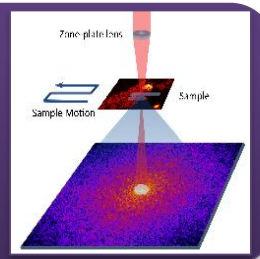
Spectroscopy
(MicroXas)

ShirleyXAS (MSD)
BerkeleyGW (NERSC)



Hybrid
(COSMIC)

Ptychographic
reconstruction

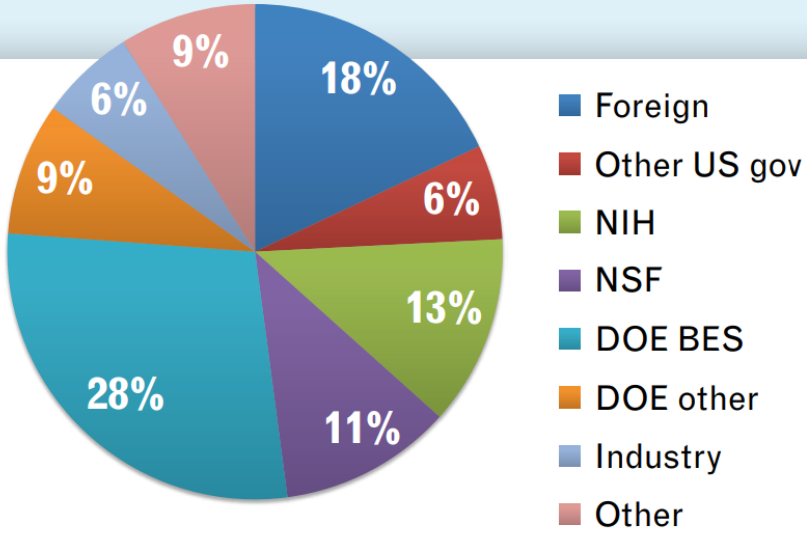


USER STATS

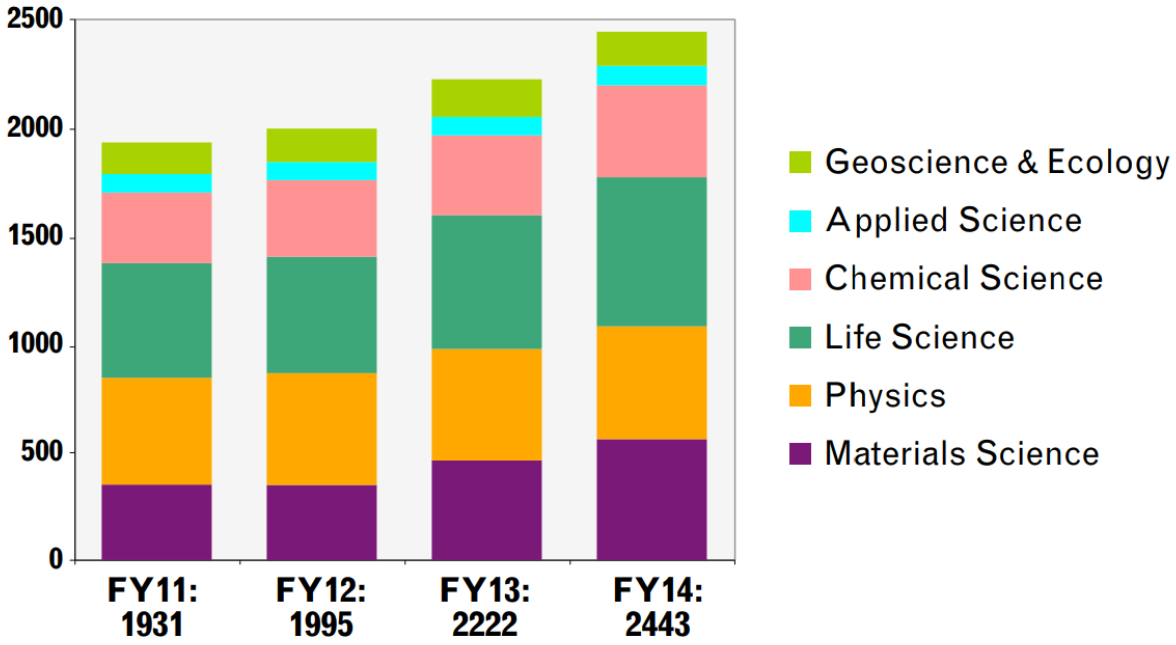
50-100
Users on site at any one time

1 hour to 10 days
Average stay of users

Users by Funding

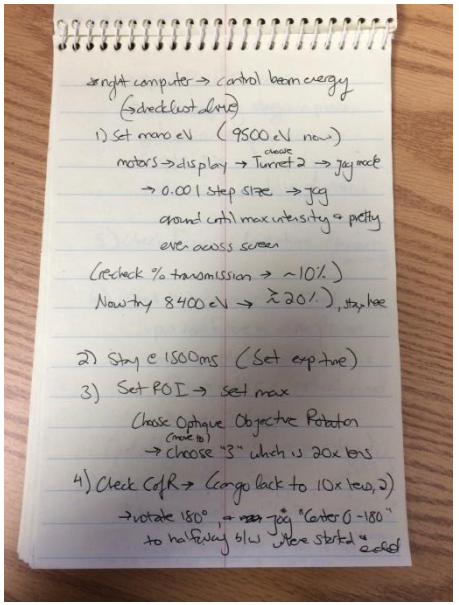


Users per Discipline per Fiscal Year
(includes remote users)



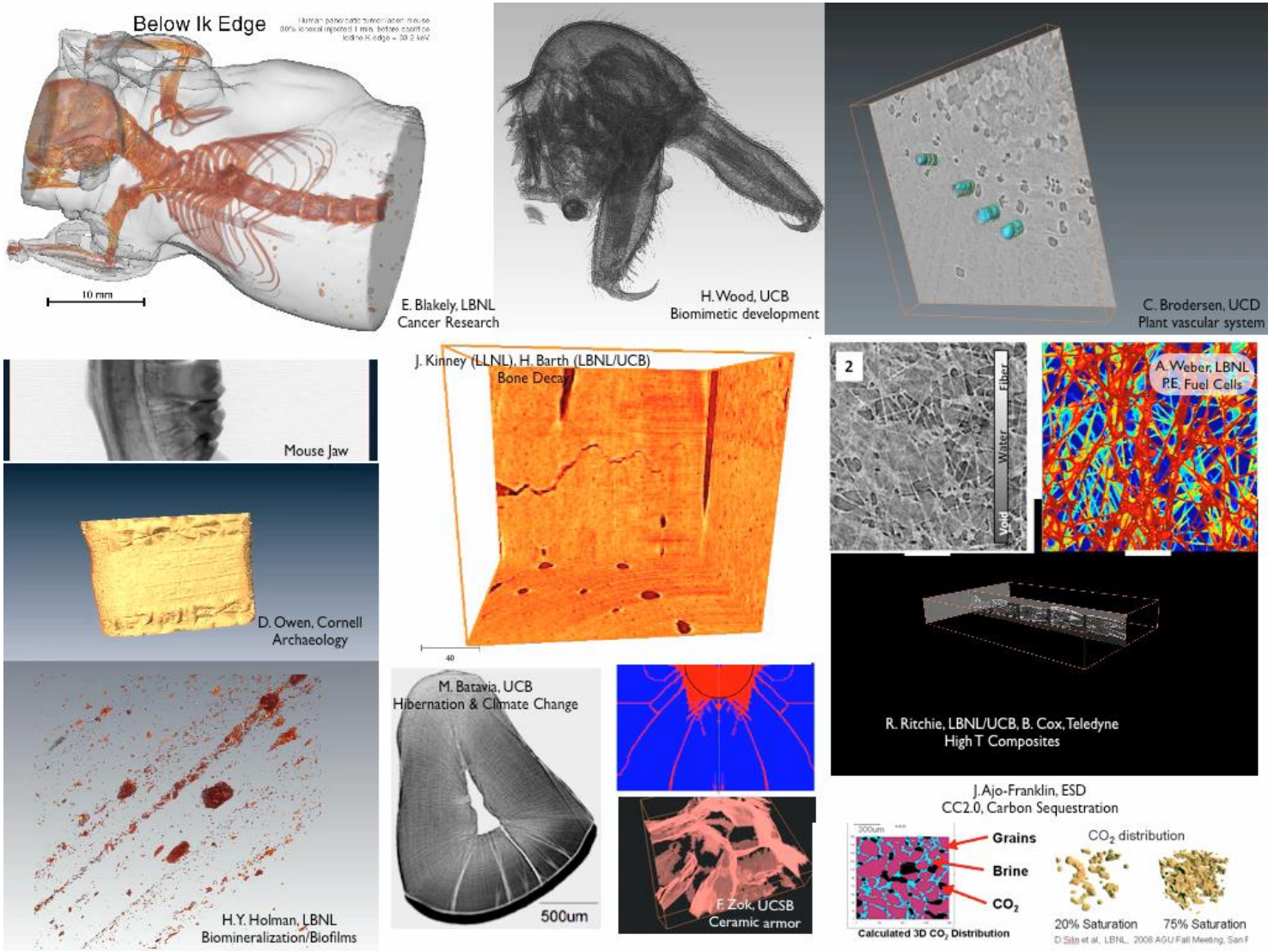
Day In the Life of a New User

- PI's, postdocs, grad students, undergrads, technical staff, industry
- Schedule
  - 9:00 – 10:00: safety, orientation
  - 10:00 – 12:00: set up first scan
  - 1:00 – 3:00: first processing using new software
  - 3:00 – 6:00: troubleshoot
  - 6:00-> on their own
- Repeat in 6 months



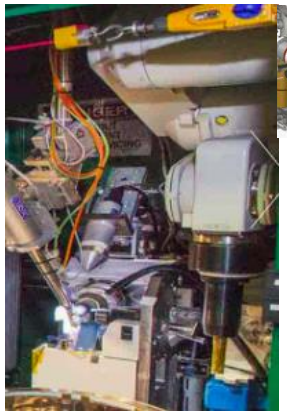
User's notes and phone video

Huge variety: This slide is a selection of experiments from 1 of 40 beamlines at 1 light source…



Increasing data rates and computing complexity are driving interest in computing beyond what can be done at beamline

Robots



BL5.0.2

MAESTRO

BL7.3.3

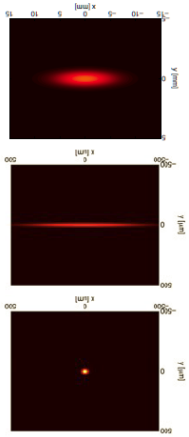
Detectors

BL7.3.3
Pilatus 2M
10Gbps

5.3.2.1 Fast CCD
>6 Gbps

BL 8.3.2
PCO Dimax, 5 Gbps

Brightness

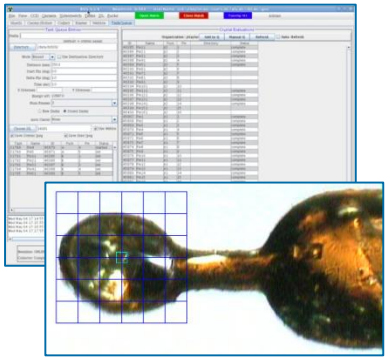


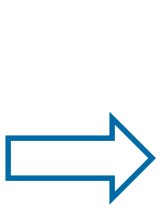
ALS

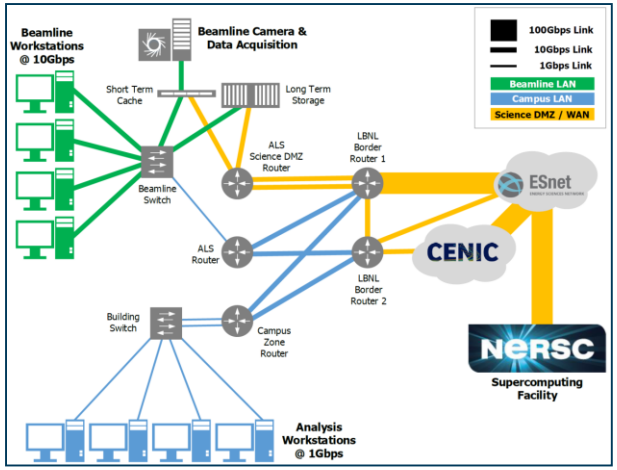
ALS lattice upgrade

ALS-U

Software/ Automation



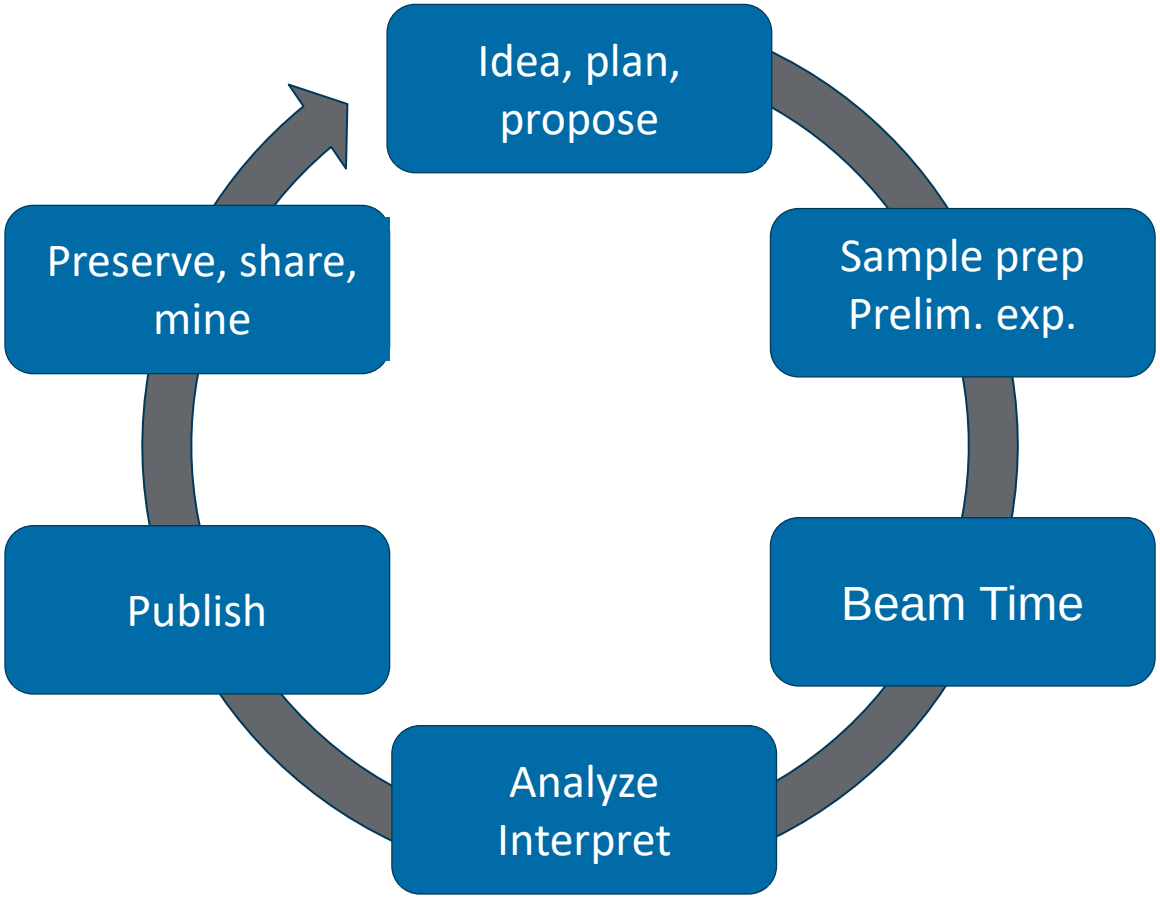




Distributed Computing/ Virtualization Needs

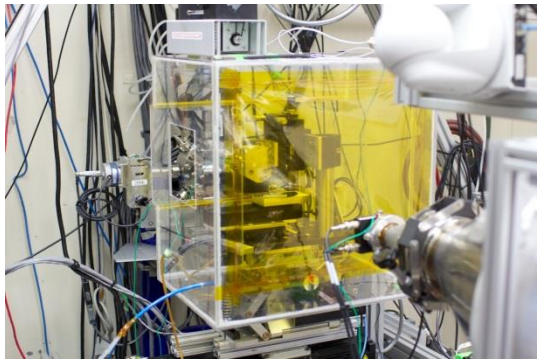
- Increasing need for more (or different) compute capabilities than exist at the beamline or light source
- Uptime is critical
  - During beamtime, need feedback for experiment
  - Always want access to database/portal even if data/compute isn't available
  - Dynamically deploy on necessary/available resources to match needs
- Build once, deploy many times
  - Deploy data ingestion system at MANY instruments
  - Deploy data access / analyze / visualize / manage—make it equally easy for users to have tools on our computers or their own.

Superfacility for User Science Before, During, and After Beam Time



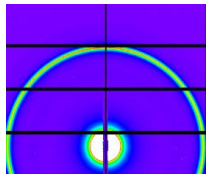
SPOT Suite Data Demo (Hexemer, Tull)

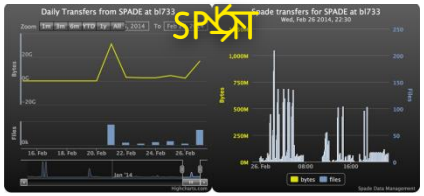
Collect data at 7.3.3



Transfer to NERSC

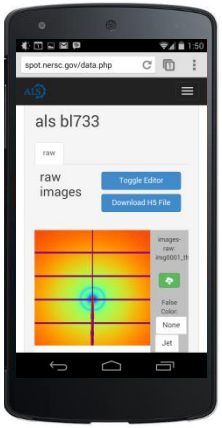
Pre-Process





Launch job at TITAN

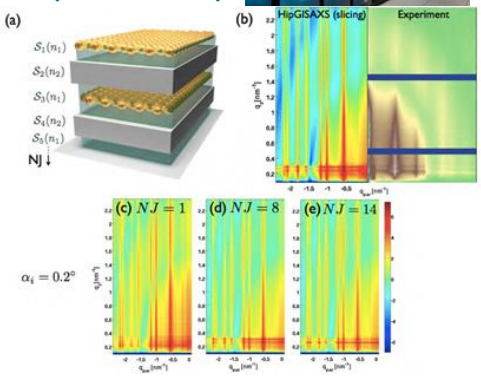
Launch job at NERSC



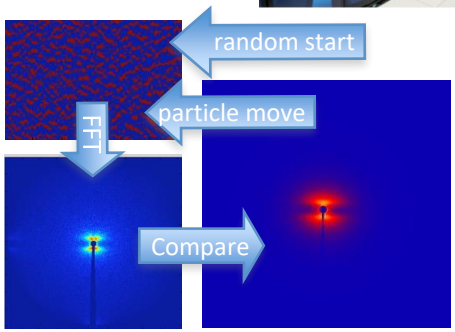
View Results Anywhere

SPOT Manages Data Transfer, Workflow, and Presentation

HipGISAXS (CAMERA)

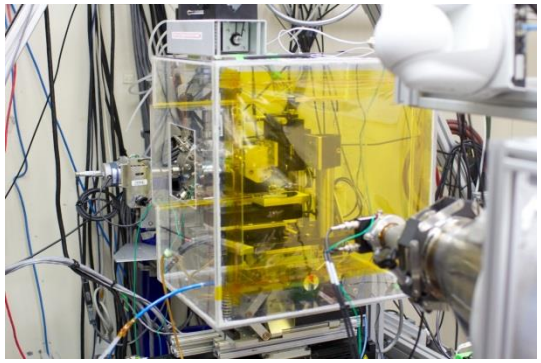


HipRMC



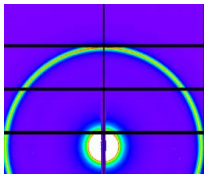
SPOT Suite Data Demo (Hexemer, Tull)

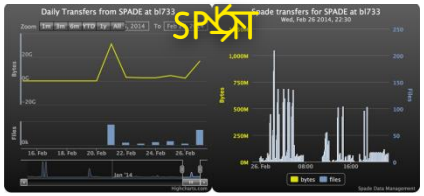
Collect data at 7.3.3



Transfer to NERSC

Pre-Process





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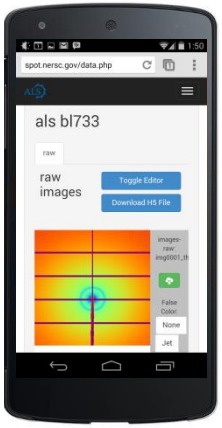
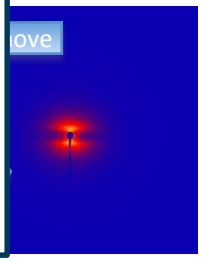


View Results Anywhere

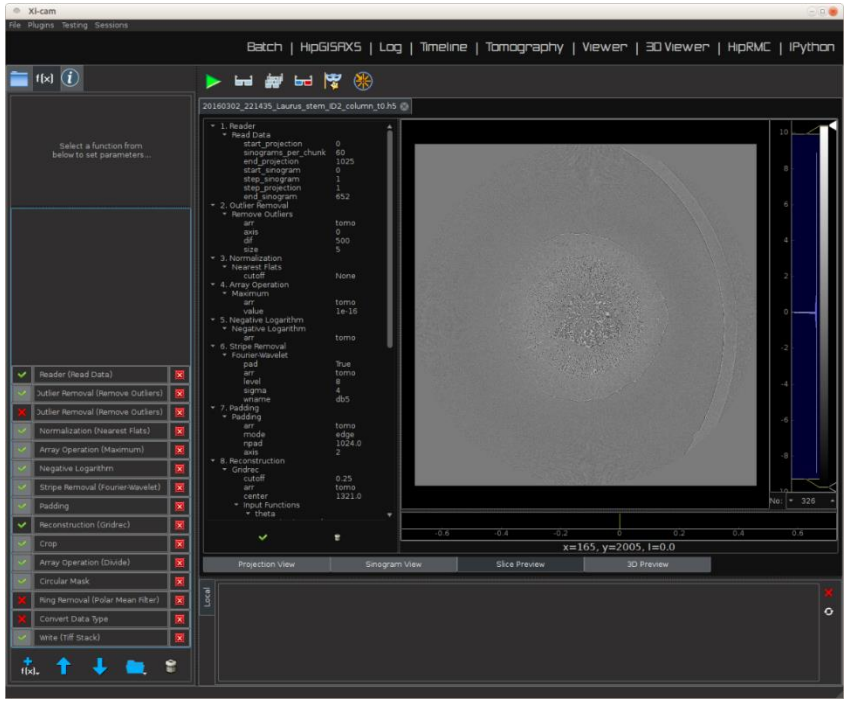
SPOT Manages

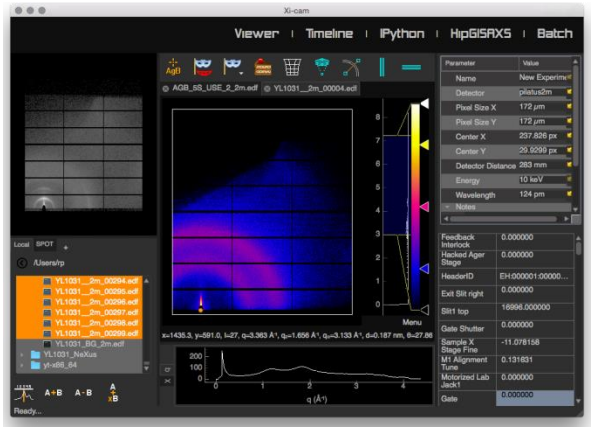
Looking forward to using NERSC's SHIFTER and SPIN!



Xi-CAM Analysis Interface

- Plugin architecture
  - Scattering
  - Tomography
  - Easy to add more
- Data and computation can be local or remote





Developed by CAMERA Applied Math

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