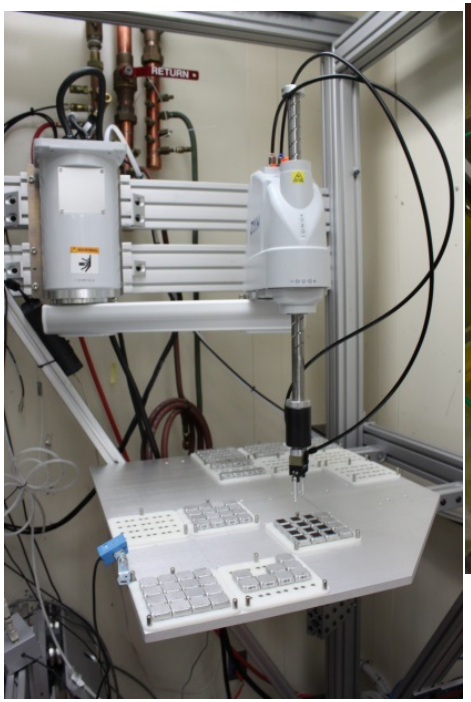
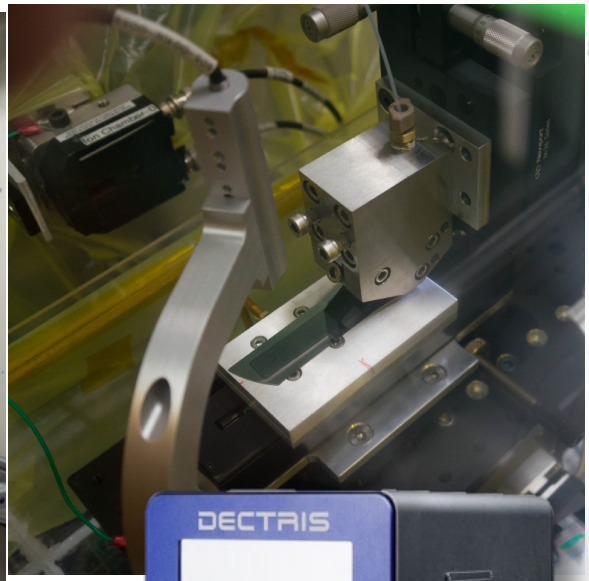
High Performance Computing for Synchrotrons

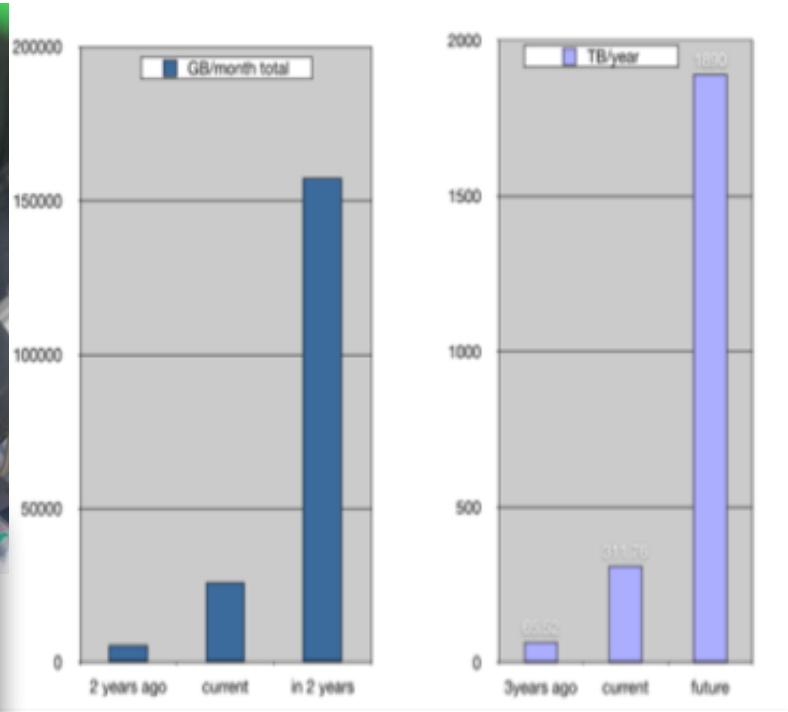
Alexander Hexemer

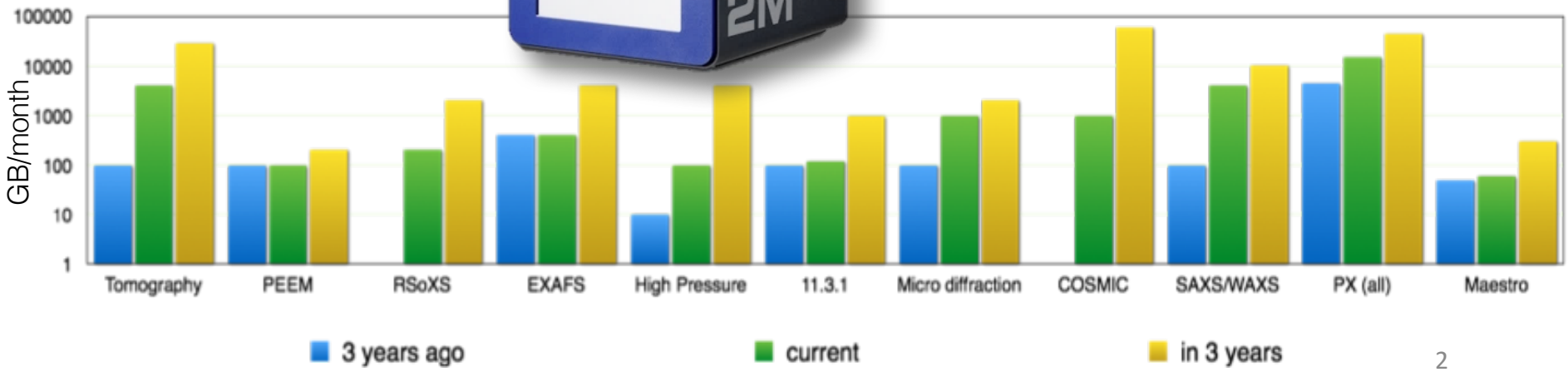
Advanced Light Source, Lawrence Berkeley National Laboratory

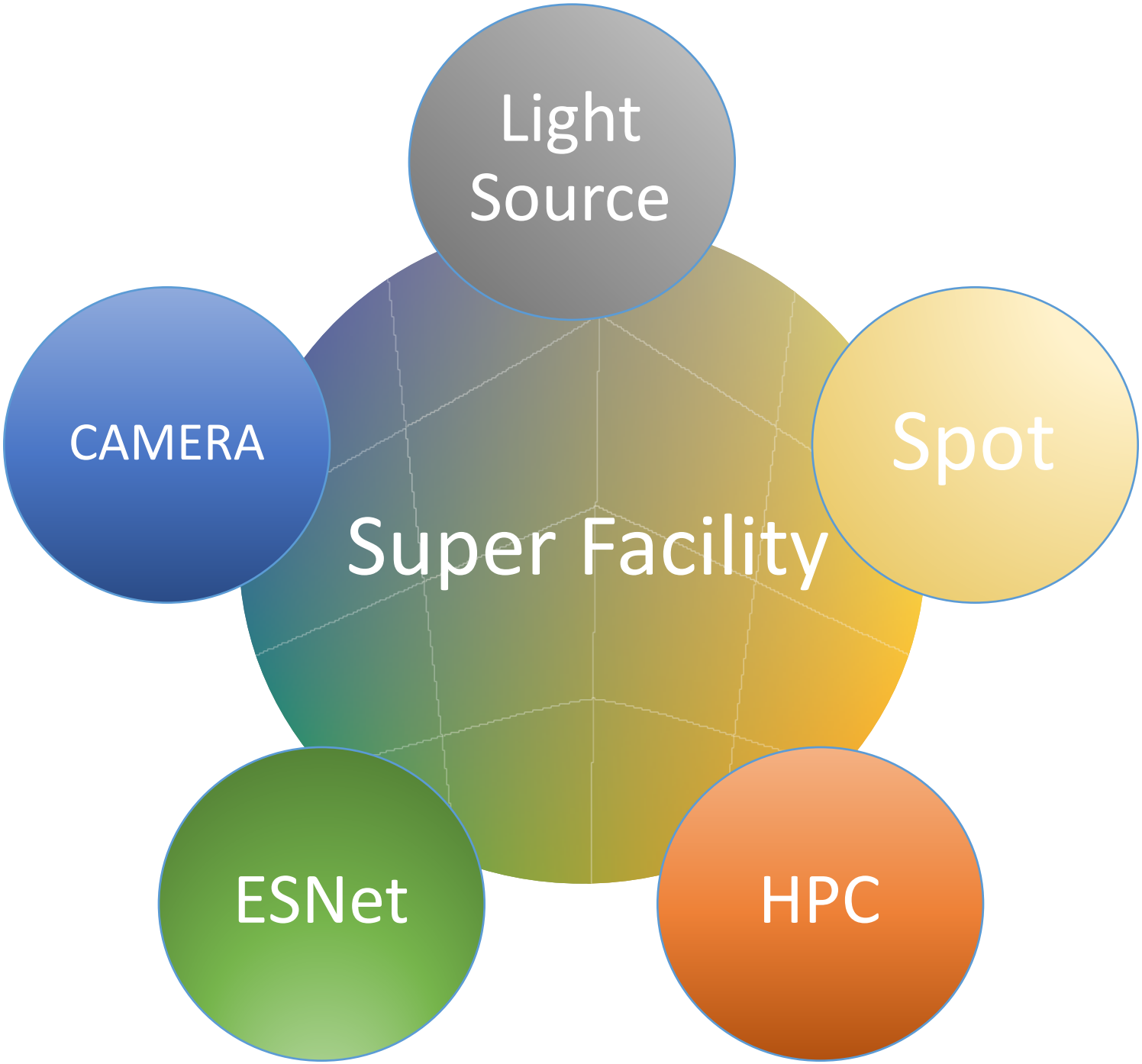
2 Petabytes/year of raw complex data.





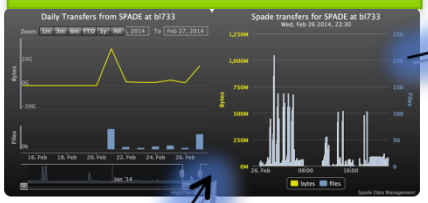




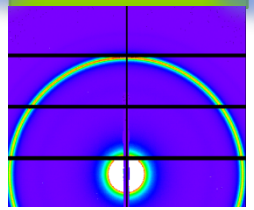

Light Source
CAMERA
Spot
Super Facility
ESNet
HPC

Data Flow

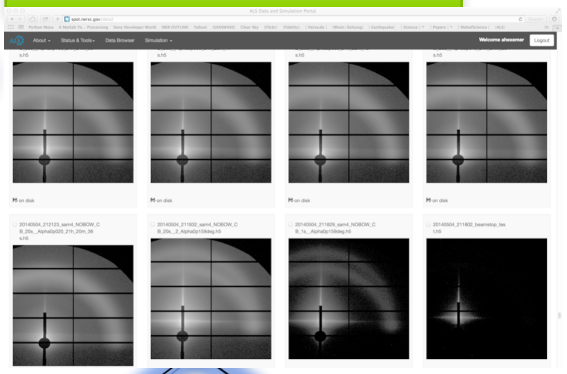
Transfer to NERSC



On-the-fly calibration, processing

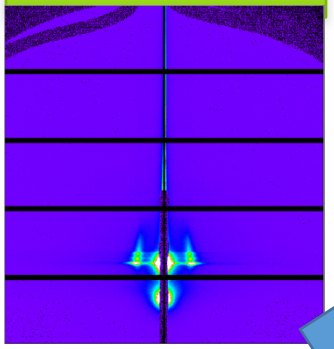


Real-time access via web portal



Combining:
GIXSGUI, dpdak + …

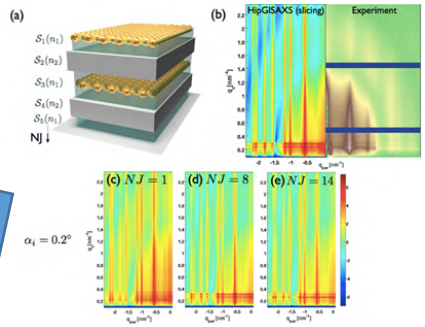
Data collection

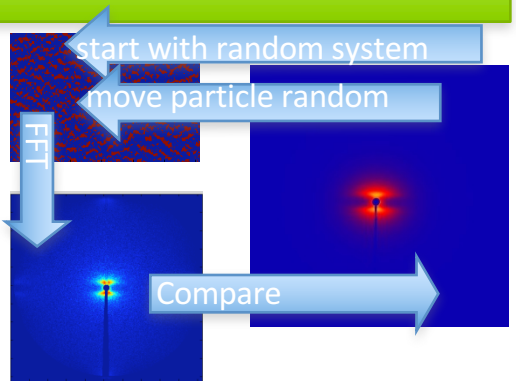


Analysis and modeling on NERSC supercomputers:

HipGISAXS simulation

HipRMC fitting





Autotuning

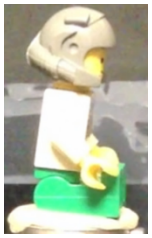
ALS Data Portal

POWERED BY

NERSC ESnet CRD

Tomography Pipeline

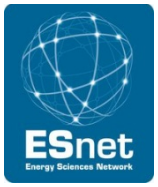
Prep Sample



X-ray Image

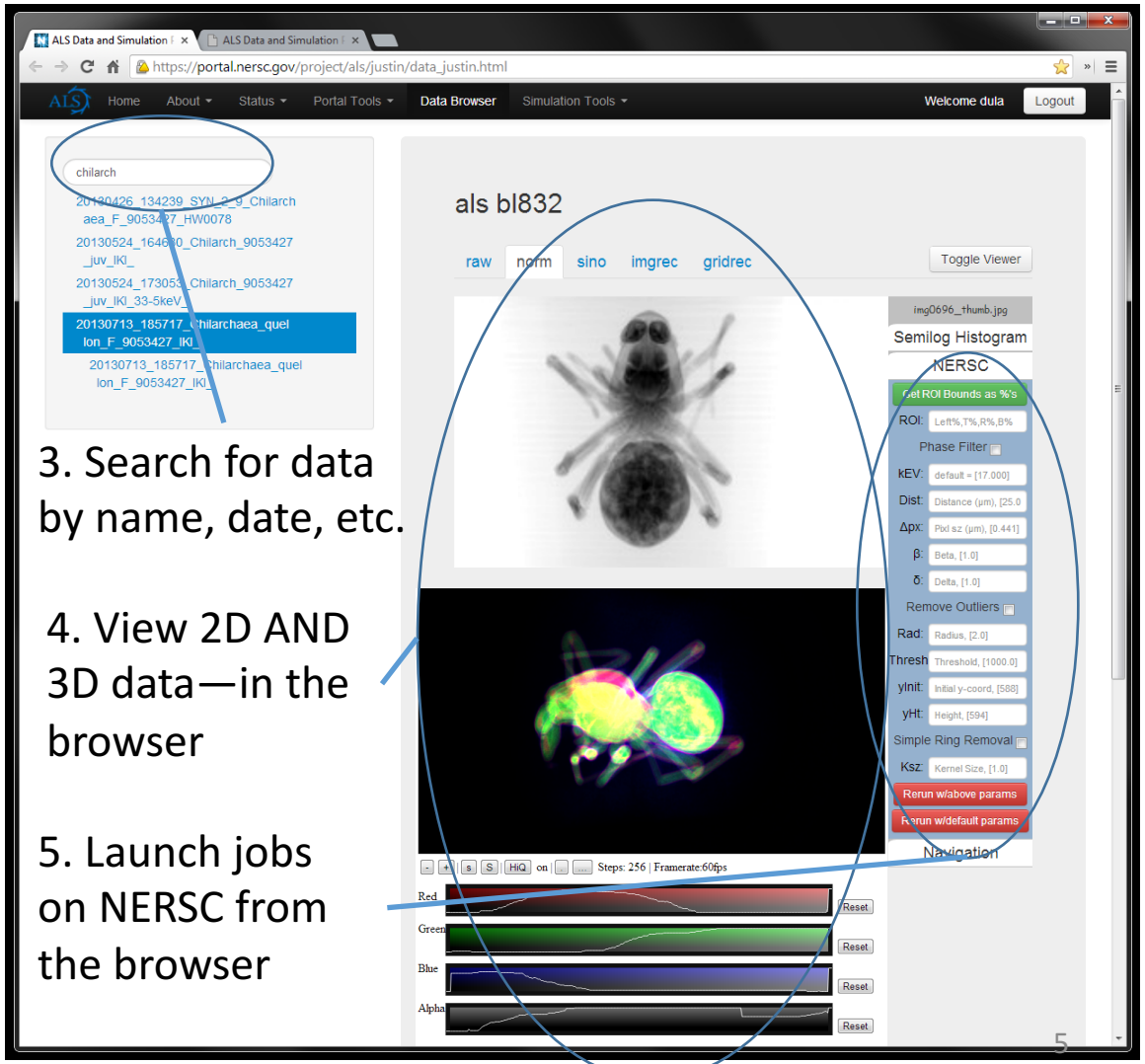
Store/ Pack Data

Move Data



Process/ Simulate

SPOT FRAME-WORK



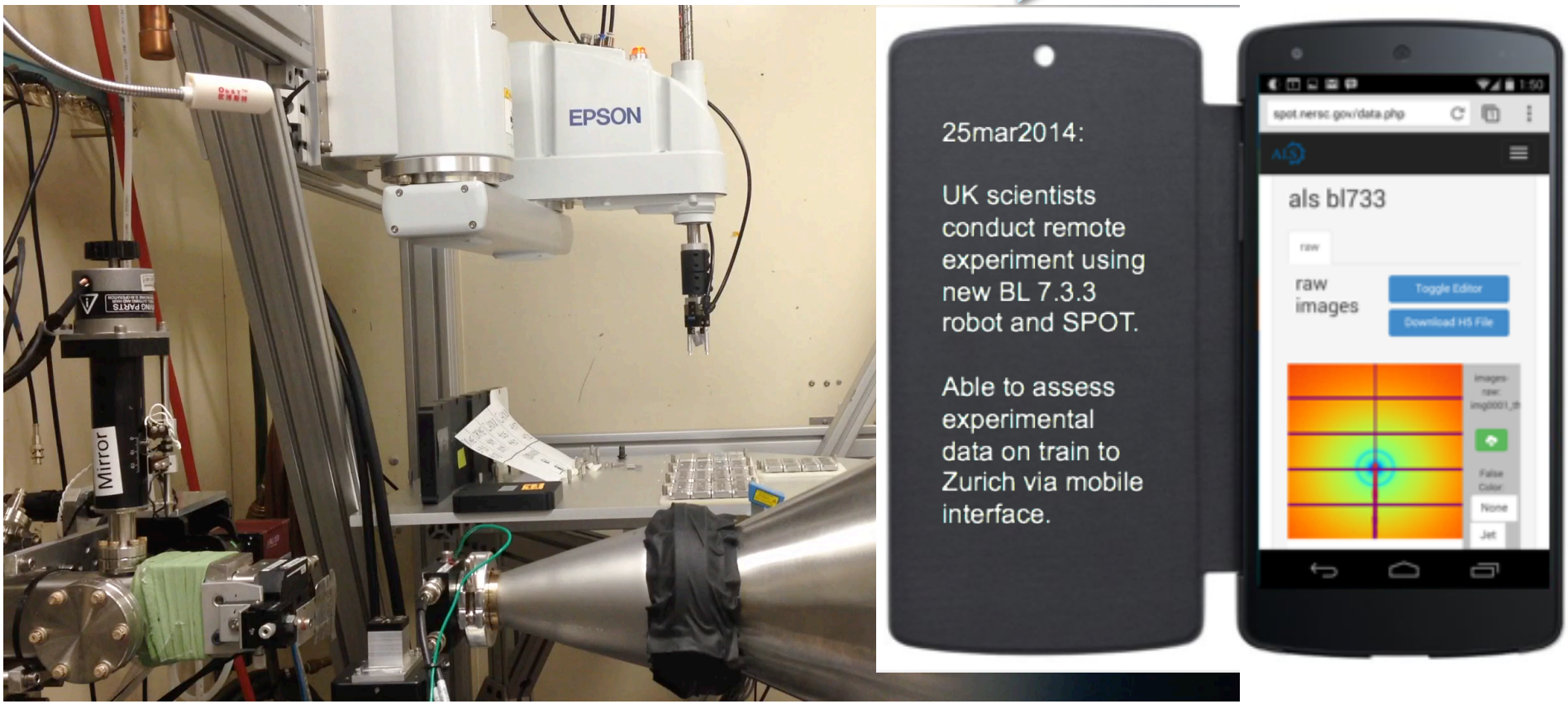
3. Search for data by name, date, etc.

4. View 2D AND 3D data—in the browser

5. Launch jobs on NERSC from the browser

Data movement and access

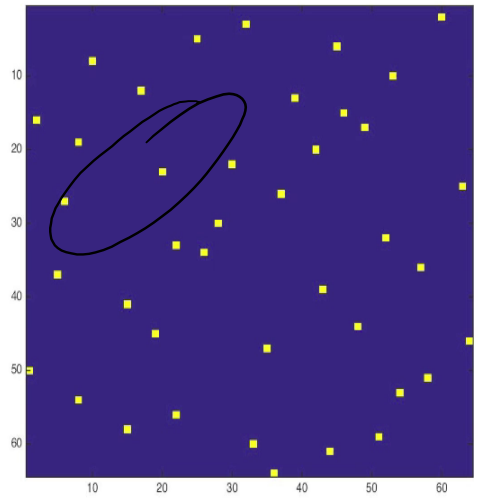
ALS → ESNET → NERSC



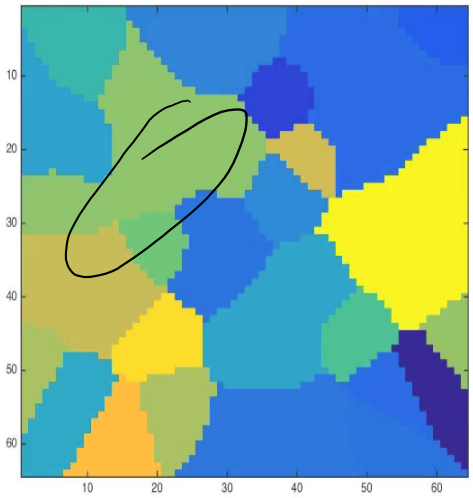
From User: Alessandro Sepe as2237@cam.ac.uk -- "Actually, I did not feel any difference between a standard beamtime and this NERSC remotely accessed beamtime, which is quite an extraordinary result"

Dynamic Image Sampling

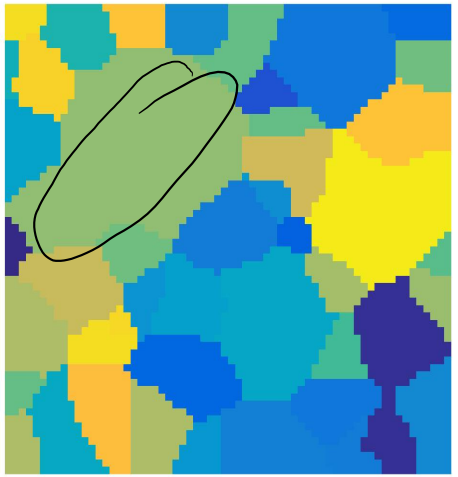
Measurement Locations



Reconstructed Image



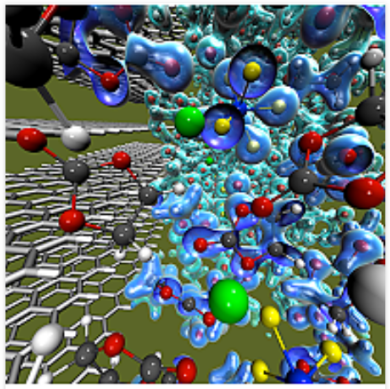
Original Image **(Target)**



G. M. Dilshan Godaliyadda, Gregory T. Buzzard, and Charles A. Bouman, ``A Model-Based Framework for Fast Dynamic Image Sampling,'' {IEEE International Conference on Acoustics Speech and Signal Processing,}

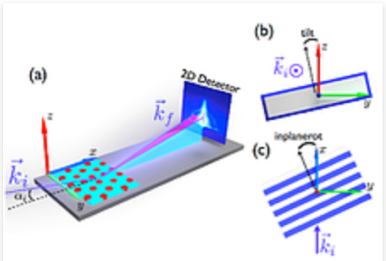
Center for Advanced Mathematics for Energy Research Applications

CAMERA Applied Math

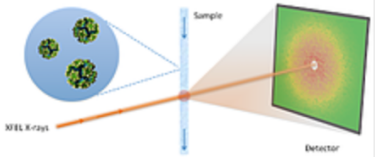


Electronic Structure

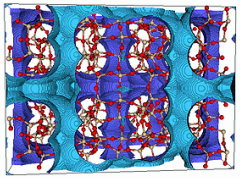
Nanocrystallography



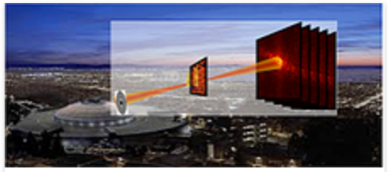
GISAXS



Fluctuation Scattering



Material Informatics



Ptychography

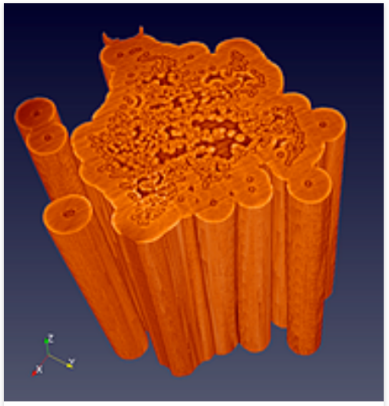


Image Analysis

Jamie Sethian
Head of CAMERA

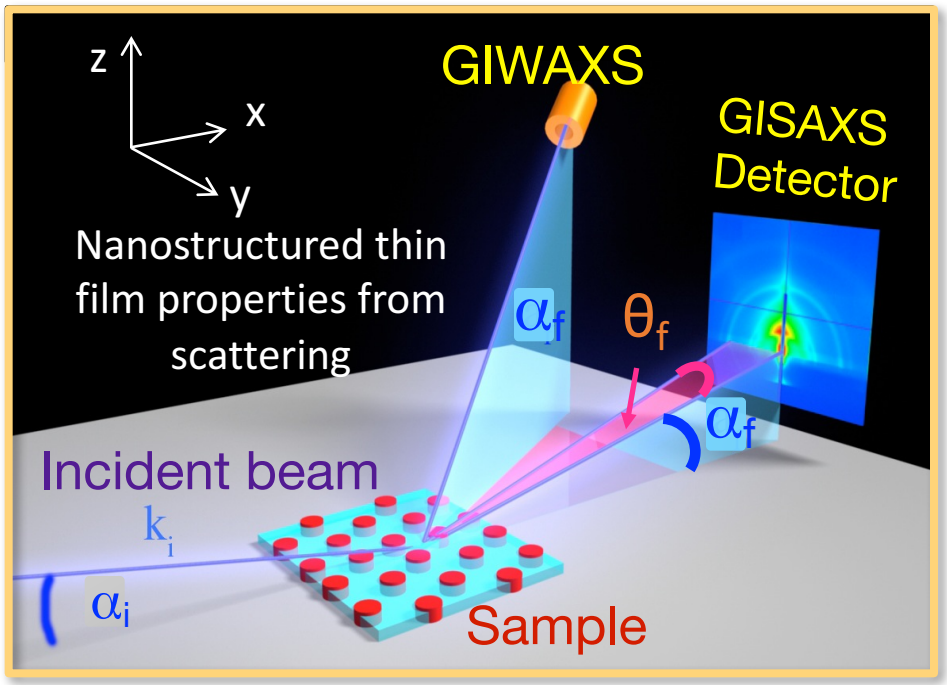
DOE: BES and ASCR

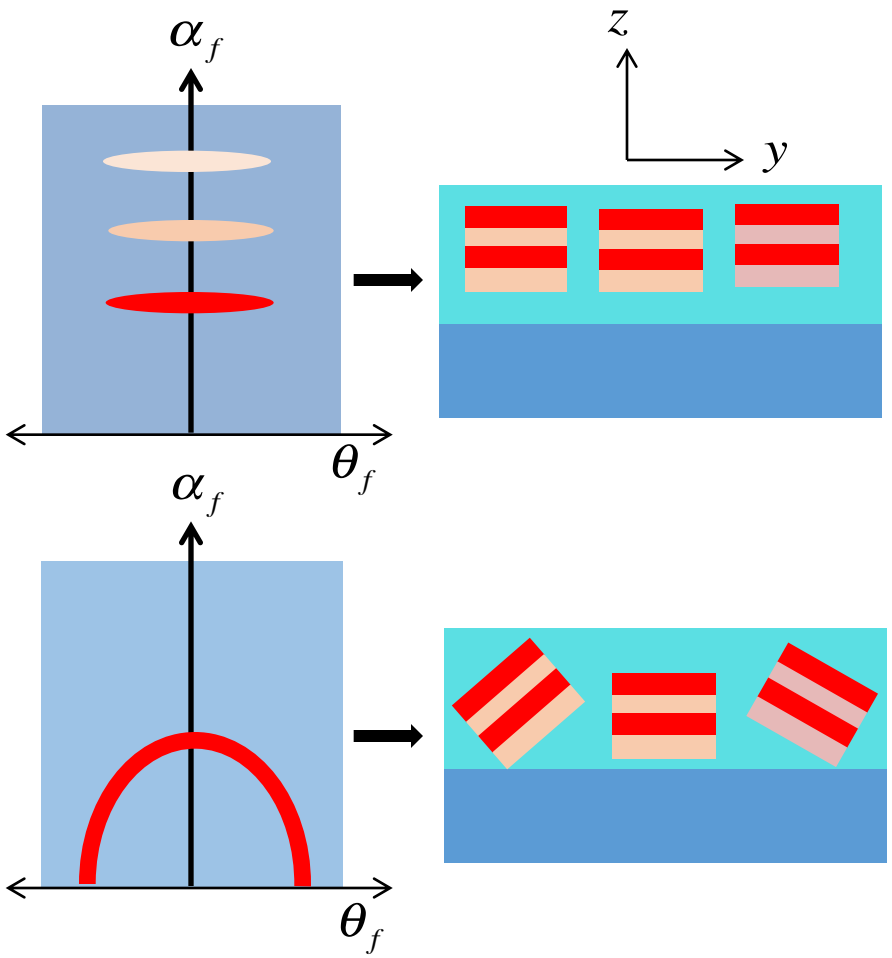
$10.5M for 3 years

Include latest theory and math, take advantage of latest architecture: Multi CPU/GPU, open source, everything shared, many collaborations

www.camera.lbl.gov

GISAXS

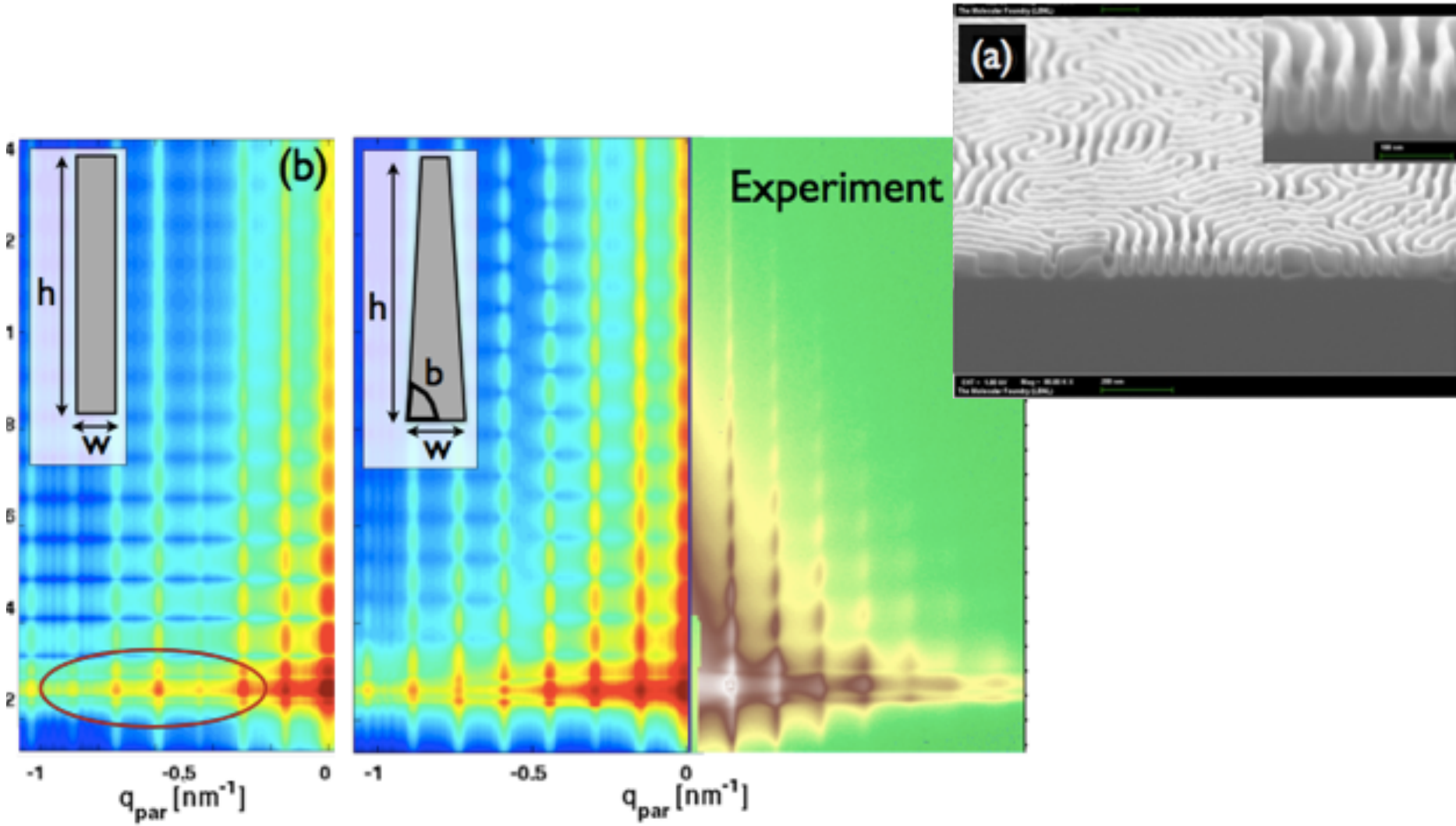




Applications : photo-voltaic, liquid crystals etc.

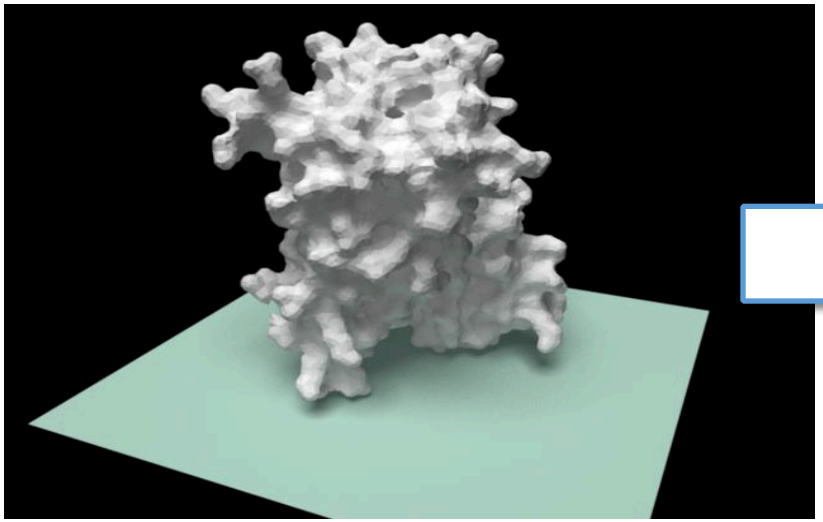
Scattering pattern gives 3-D statistical information about distribution of embedded nano-structures

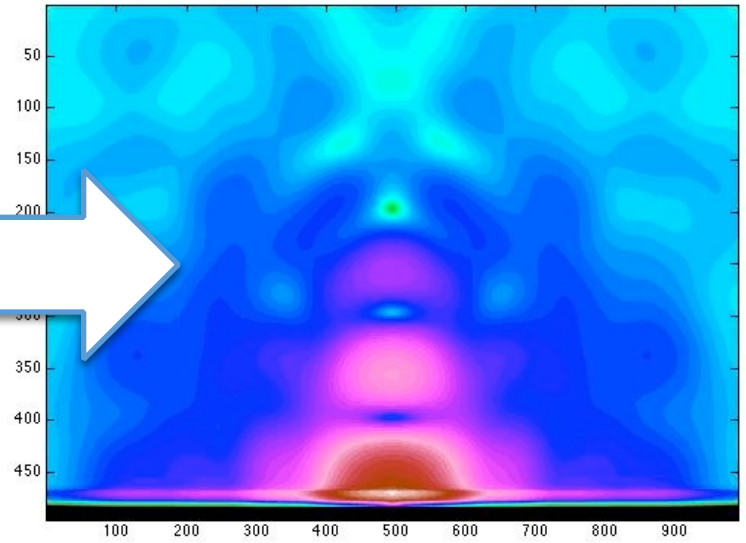
Computed GISAXS images for a "fingerprint" Si grating sample at incident angle $\alpha_i = 0.15°$



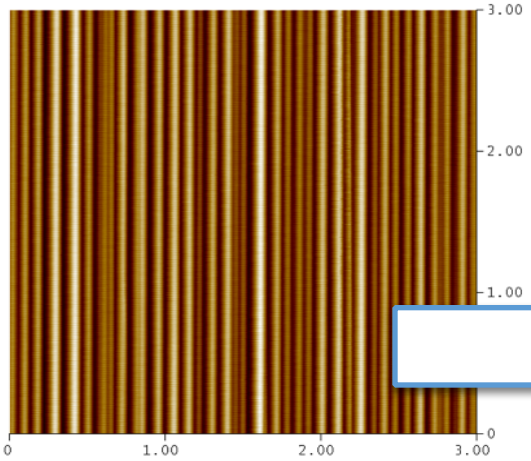
(b) Simulated GISAXS pattern for a rectangular model of the grating cross section with width and height ranges of nm and nm, respectively. (c) Simulated GISAXS pattern (*left*) using a shape with a trapezoidal cross section.

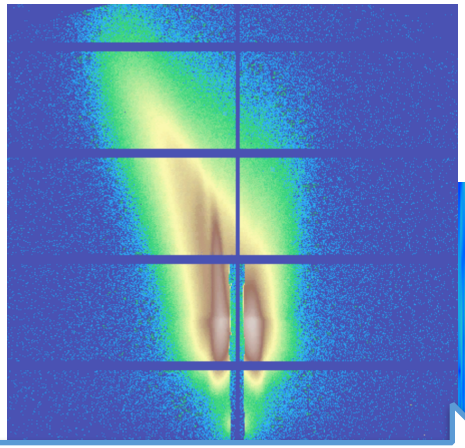
Complex Shaped

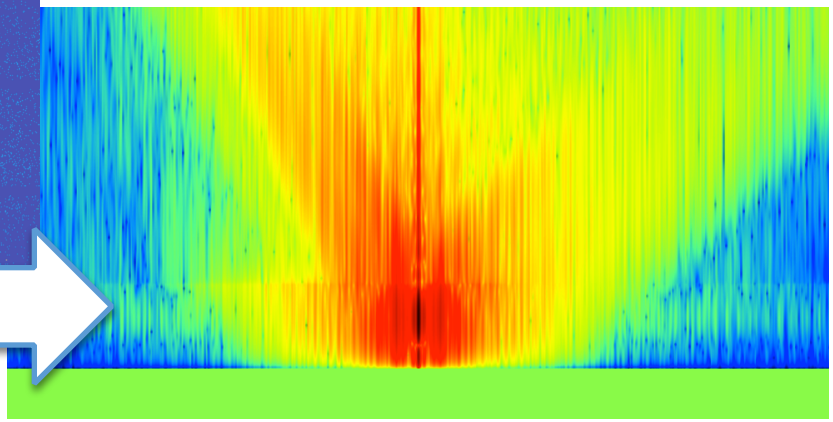


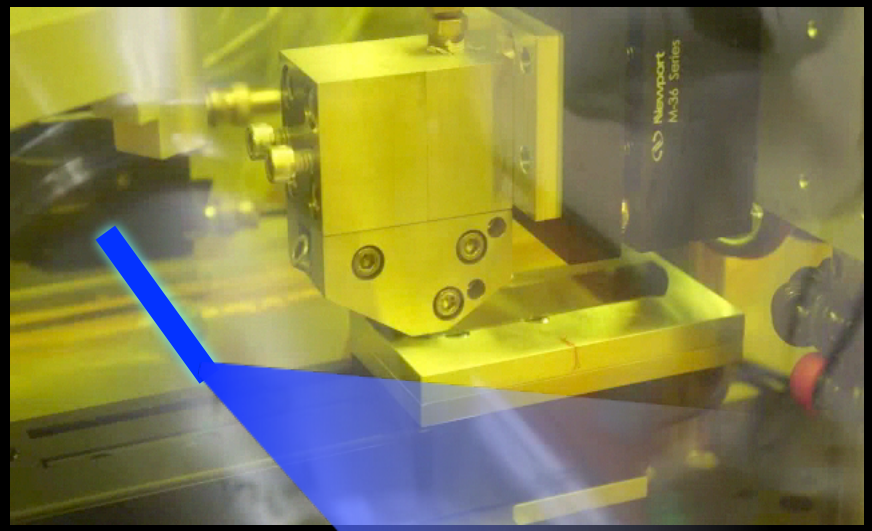


SFM image



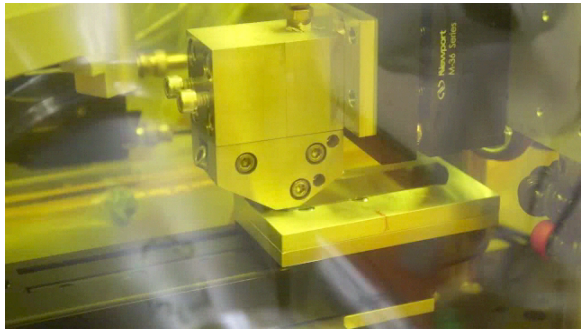


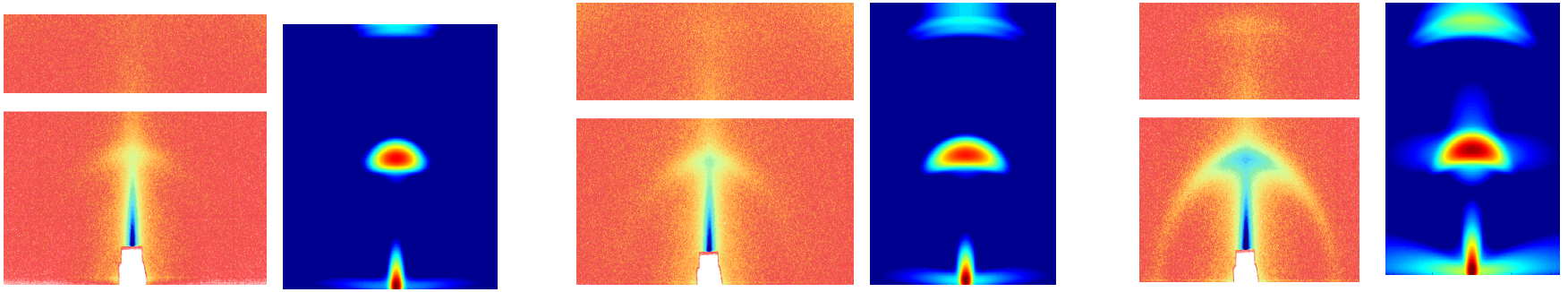




Design Model

Simulations can’t keep up





- Pre-schedule concurrent time at ALS beamline 7.3.3 and on OLCF's Titan
- Measure time-resolved scattering data of new materials
- Automatically capture metadata and transfer data to NERSC for realtime processing using SPOT Suite
- Dynamically establish a Globus Online connection between NERSC and OLCF to transfer data to and from Titan
- Automatically trigger large-scale (8,000 node) HipGISAXS computation to simulate and fit the structure to the experimental data using particle swarm optimization
- Present GISAXS fitted results and provenance through CADES and SPOT Suite.
- Display results through the web portal back to the scientists at the beamline

Xi-cam: Modular Interface for Analysis

Scientific Achievement

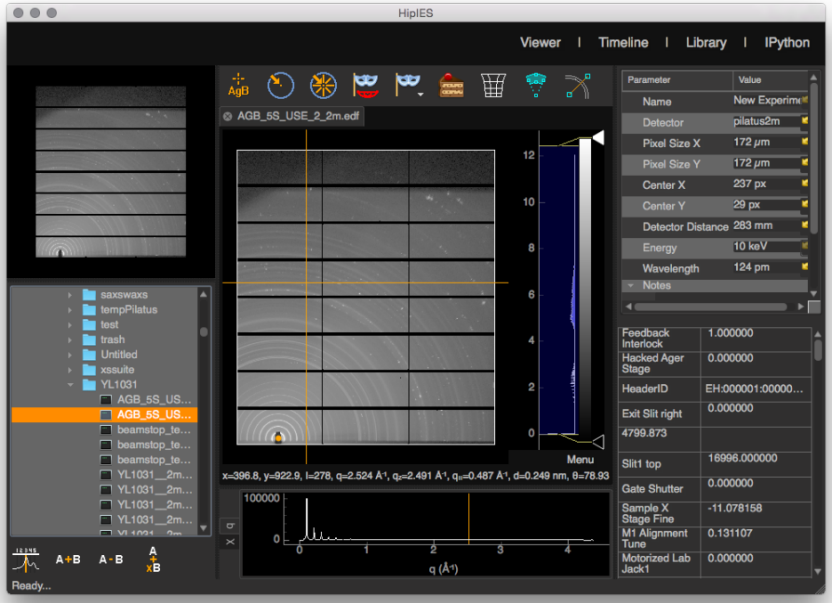
Development of a community-maintainable platform for new analysis and visualization techniques for a variety of techniques.

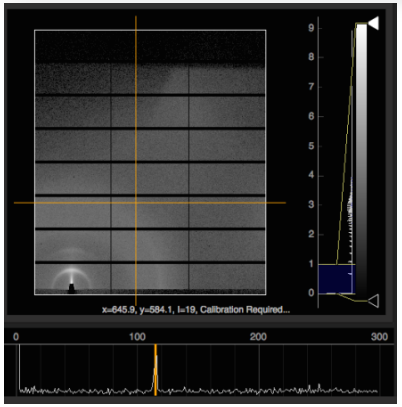
Significance and Impact

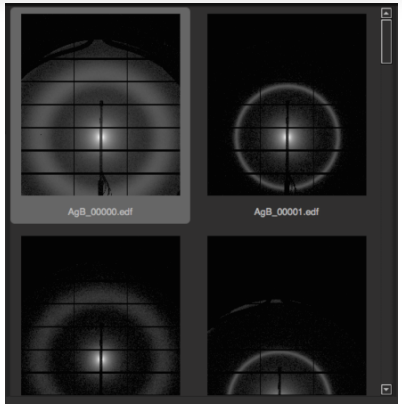
New visualization techniques extract further information from synchrotron data. Open source modular design allows collaborative development and resource consolidation across synchrotron facilities.

Research Details

- Remote processing with HPC for real-time high data rate analysis
- NERSC/SPOT remote data access for high-volume data archive retrieval (Using Globes)
- Highly interactive responsive design improves user control and accessibility







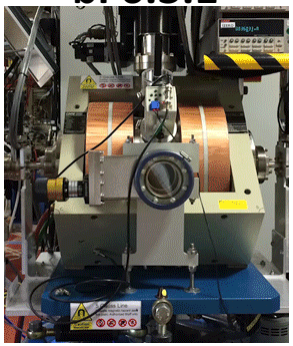
* Pandolfi, R., Venkatakrishnan, Kumar, D., Hexemer, A. *(under preparation)*

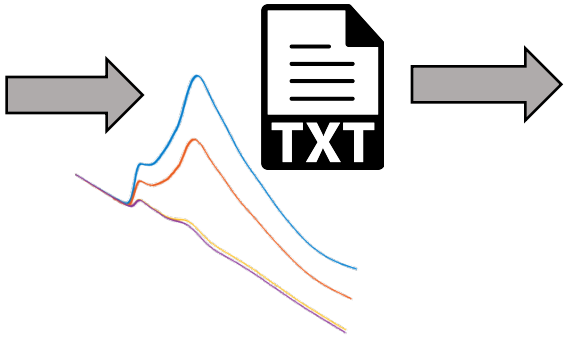
Work supported by the Early Career Award program, DOE.

The project is in collaboration between CAMERA, APS, SSRL, CFN and NSLS II.

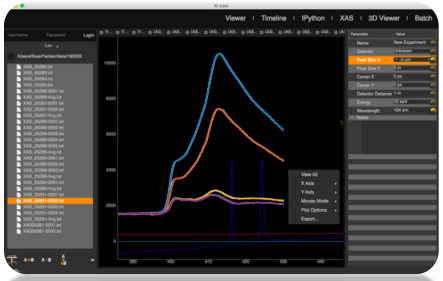
The High-throughput NEXAFS workflow

bl 6.3.1

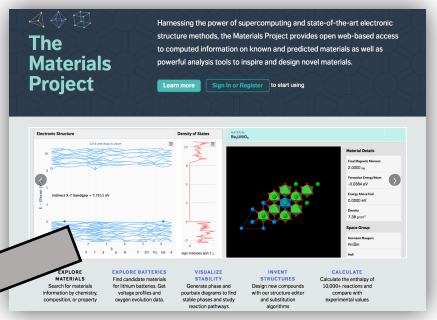




Xi-CAM Processing/reduction



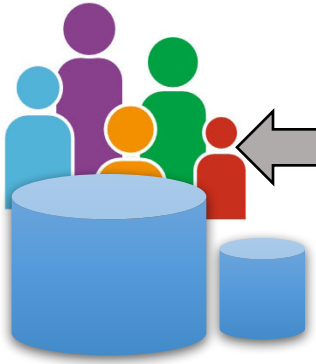
Materials Project website

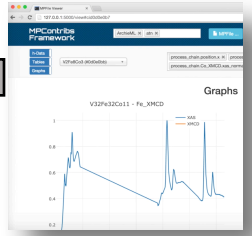


Quantities

Public

MPContribs Framework

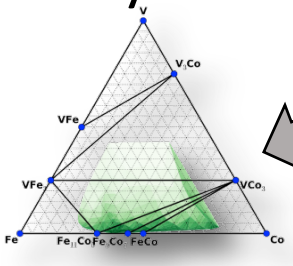




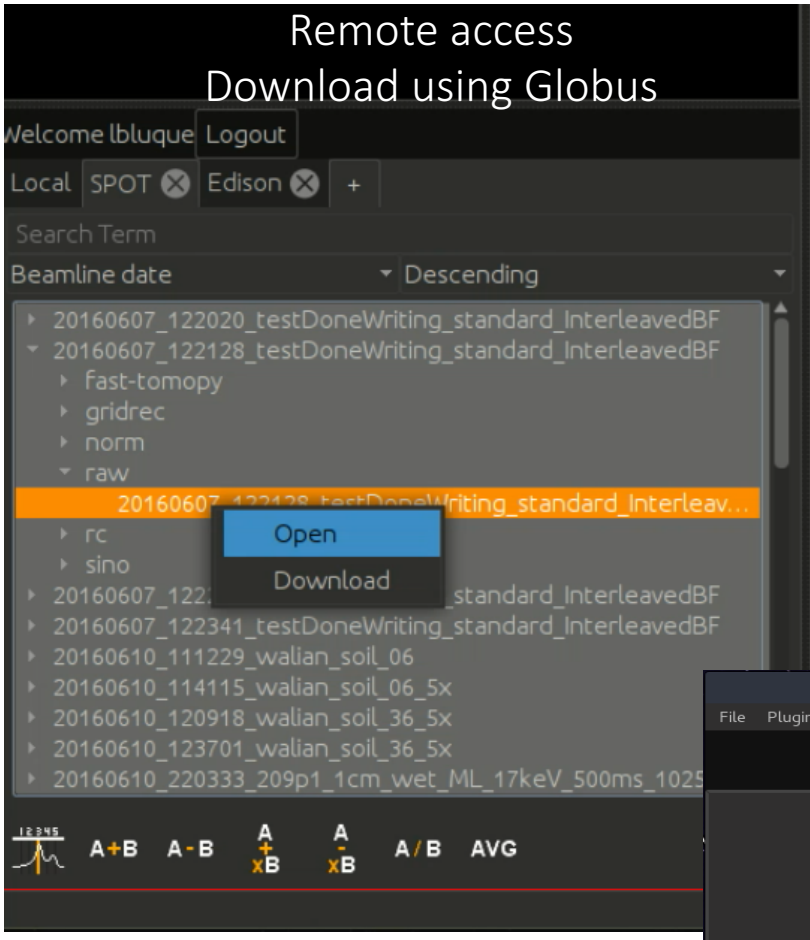
Result s

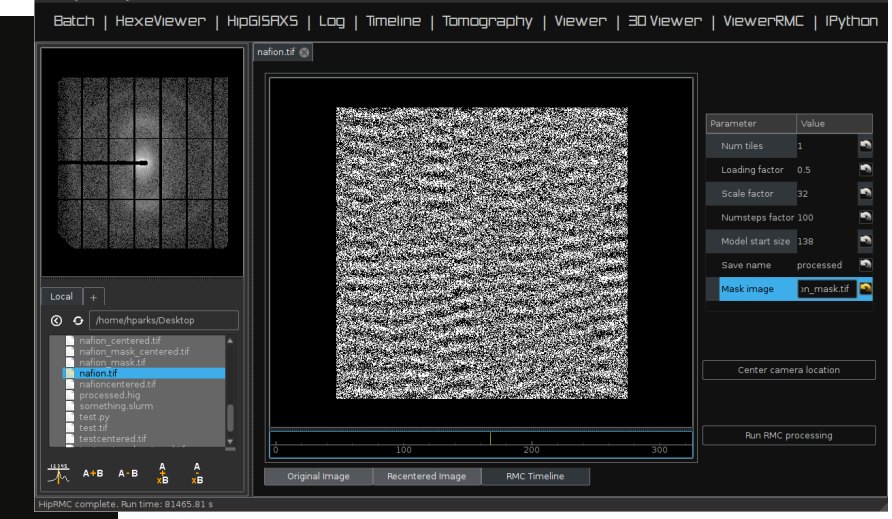
Analysis

Phase diagrams

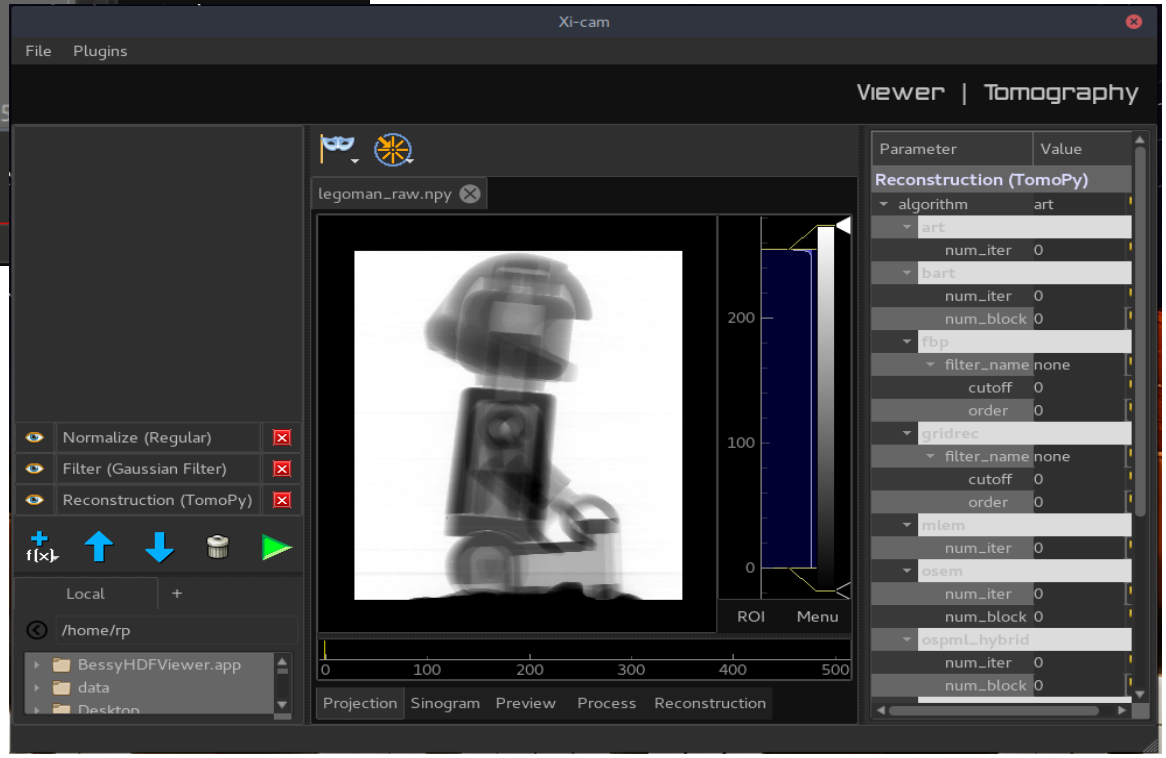


Remote access
Download using Globus

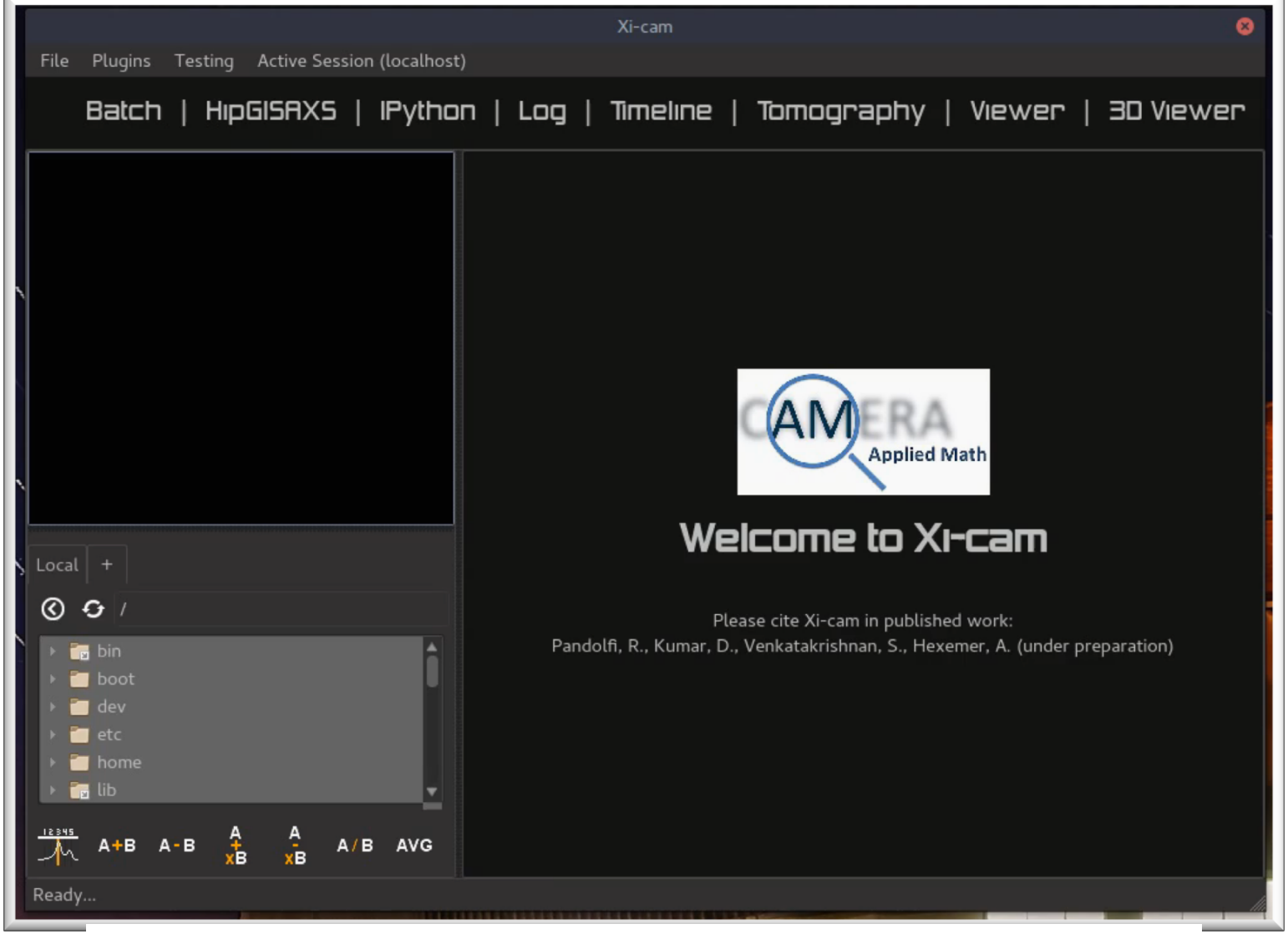




Automated reverse Monte Carlo



Tomography



adolphe merkle institute
excellence in pure and applied nanoscience

UNI FR
UNIVERSITÉ DE FRIBOURG
UNIVERSITÄT FREIBURG

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Technische Universität München

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ALS
ADVANCED LIGHT SOURCE

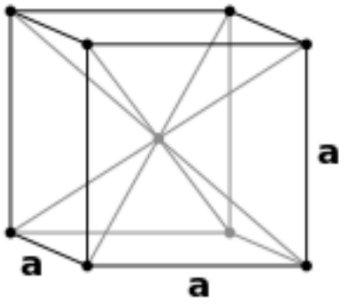
CAMERA
Applied Math

BERKELEY LAB

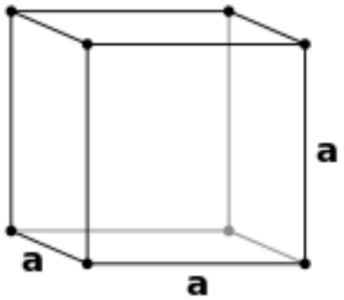
ANALYSIS: Machine LEARNING for X-ray Data

Can we classify crystal lattice from GISAXS patterns ?

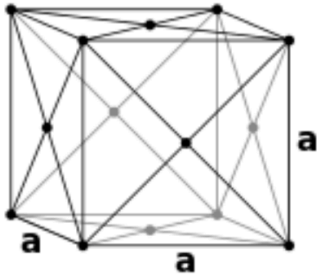
BCC



Cubic



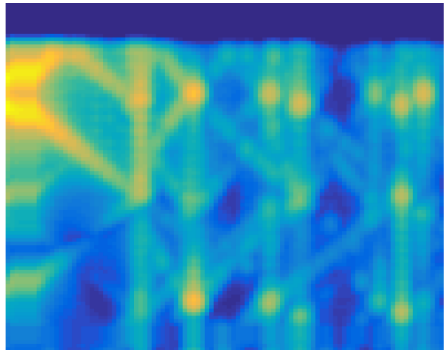
FCC



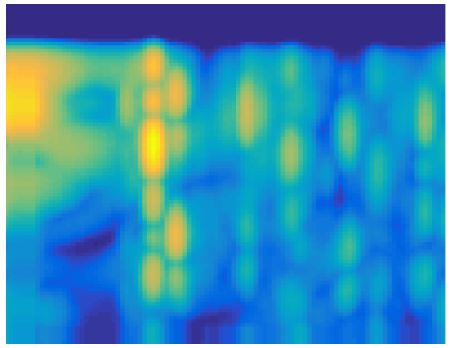
HCP

Images : Wikipedia

BCC 100



BCC 110



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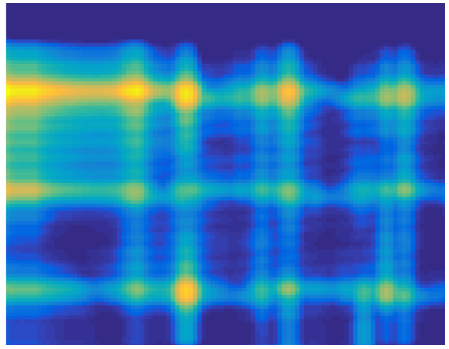

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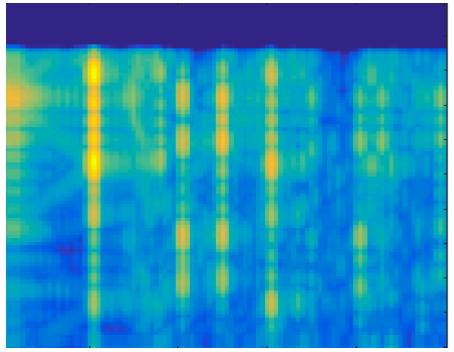

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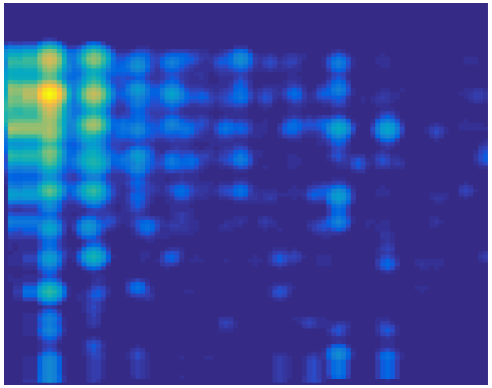

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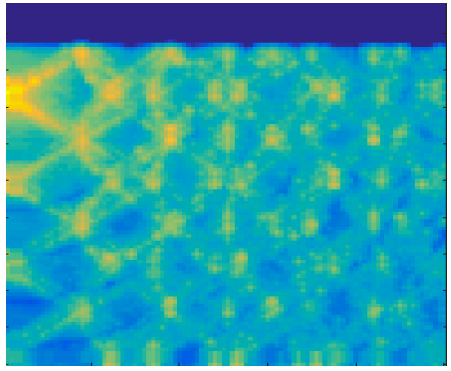

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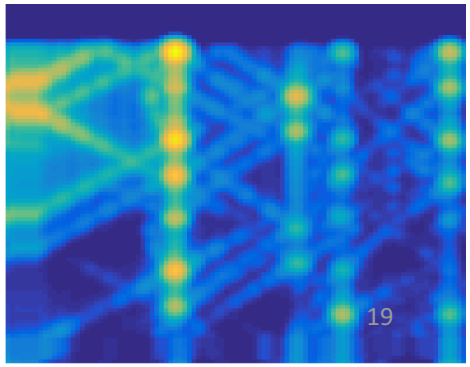
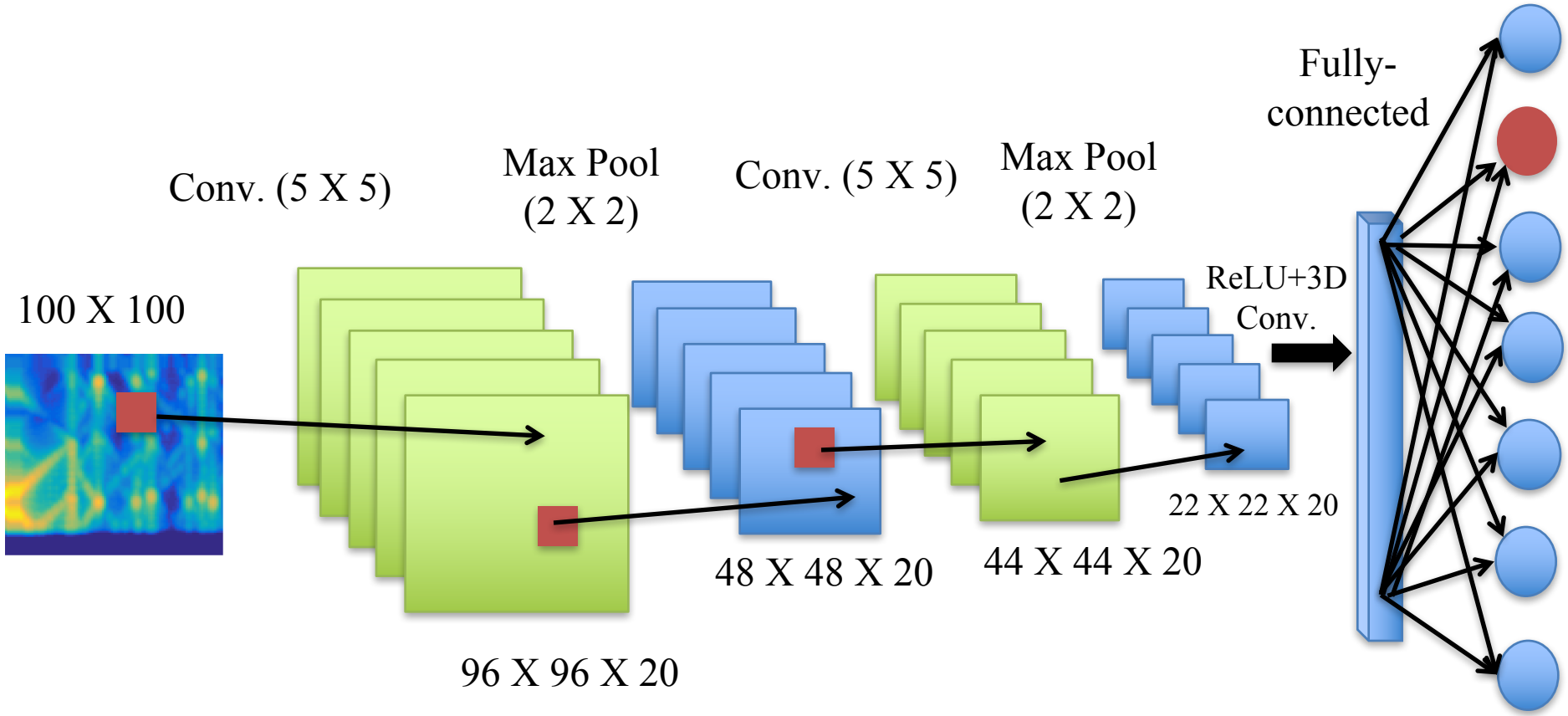


Convolutional Neural Network (CNN) - "Deep Learning" for GISAXS Image Classification*

Preprocessing: Subtract mean of training data from all inputs

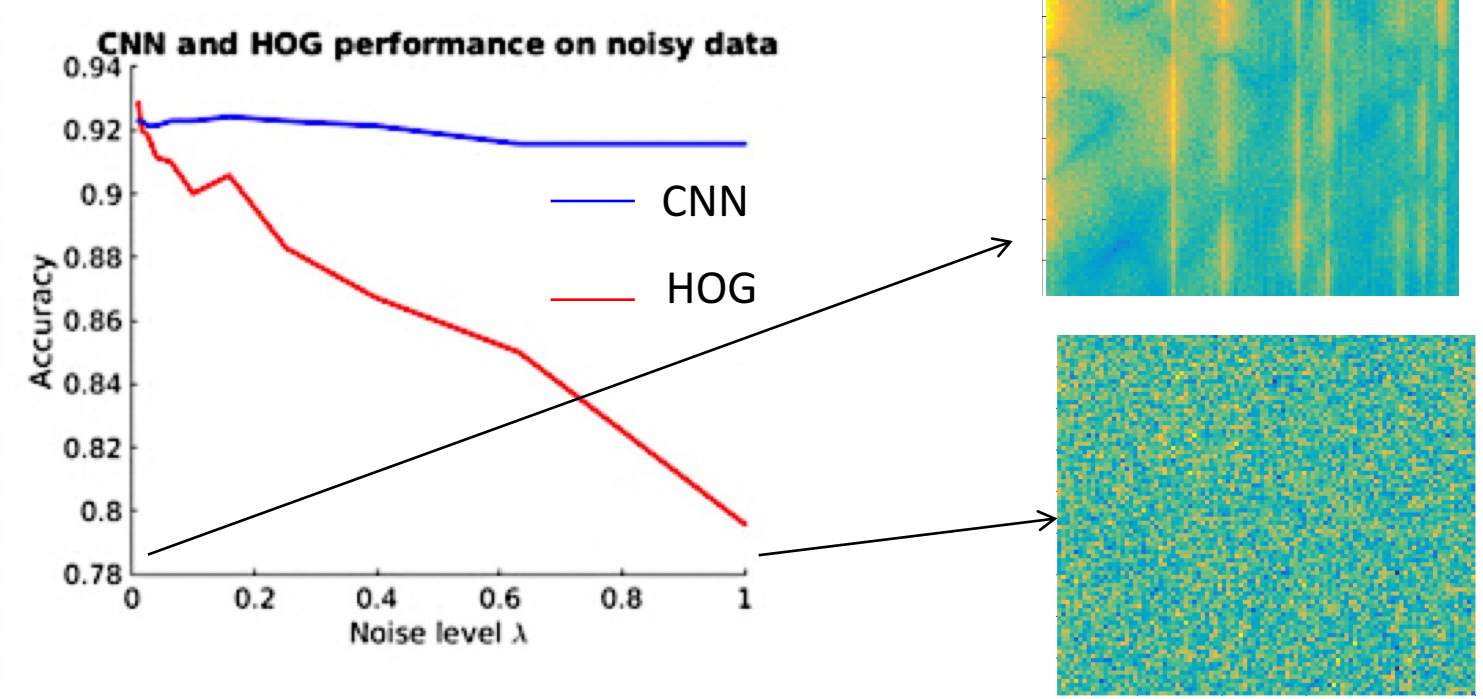
Method: Stochastic Gradient Descent with momentum



Classification Results*

Method	Accuracy: Original Data Set	Accuracy: Noisy Data
Convolutional Neural Networks (**Proposed**)	92.3%	91.6%
Histogram of Oriented Gradients (**Conventional**)	92%	80%

Deep-Learning Technique: Robustness to noise



Acknowledgements

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S.Venkat
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D. Kumar

CRD

SPOT




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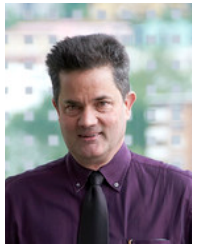
Swiss National Supercomputing Centre

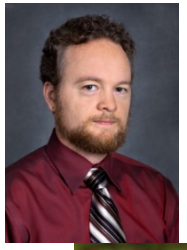
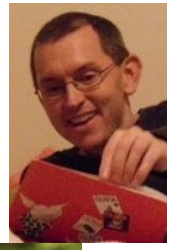



CAMERA Applied Math

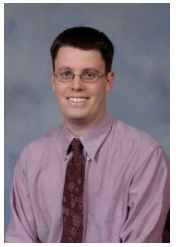



ESnet ENERGY SCIENCES NETWORK

LBLnet

NERSC

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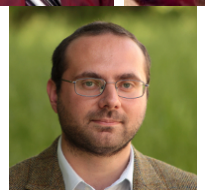

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