Superfacility: The CAMERA Project as Case Study

Special Event: Workshop on GPU Computing

Is the time your computer spends analyzing data getting out of hand? Have you heard about graphical processor unit (GPU) computing but don't know where to begin? Join us for a one-day workshop on GPU computing on July 30, 2010 in Perseverence Hall. The workshop will present an introduction to GPU computing and provide participants with an understanding of how to utilize it with little effort for their research. Speakers from Nvidia, AccelerEyes, and Tech-X will present talks on how to perform GPU computing on your machine and discuss future developments. Scientists already doing GPU computing will also present how they apply it in their work. Additional individuals who are interested in GPU computing or already have experience with it are invited to give a quick overview of their work. The workshop will conclude with hands-on computing tutorials. The event is free and individuals should register **here**. Further information may be found **here**.

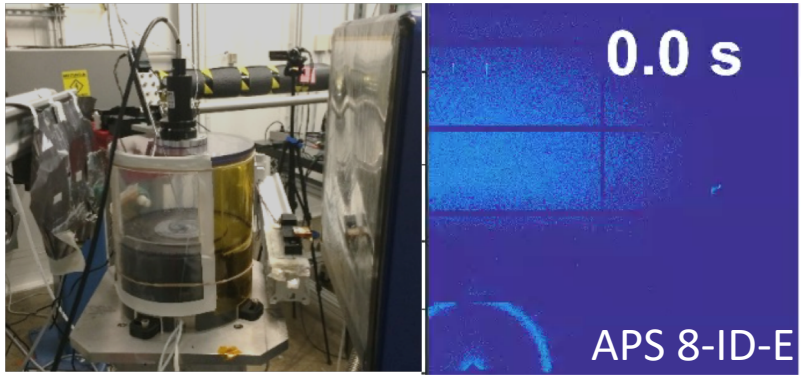
http://www.lbl.gov/Conferences/GPU/registration.html

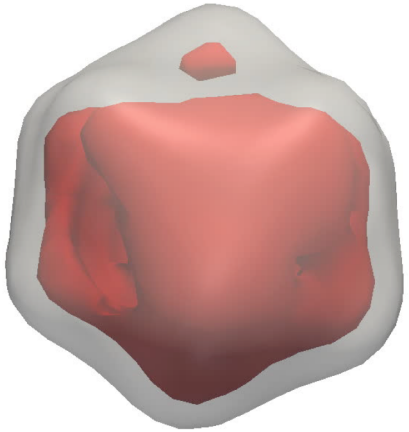
http://www.saxswaxs.com/1and1/GPU-Workshop_at_LBNL.html

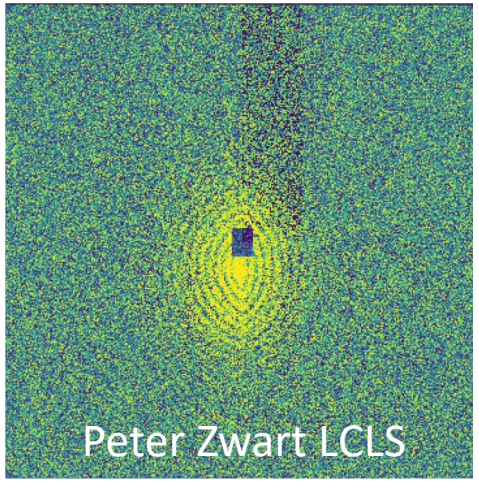
Alexander Hexemer

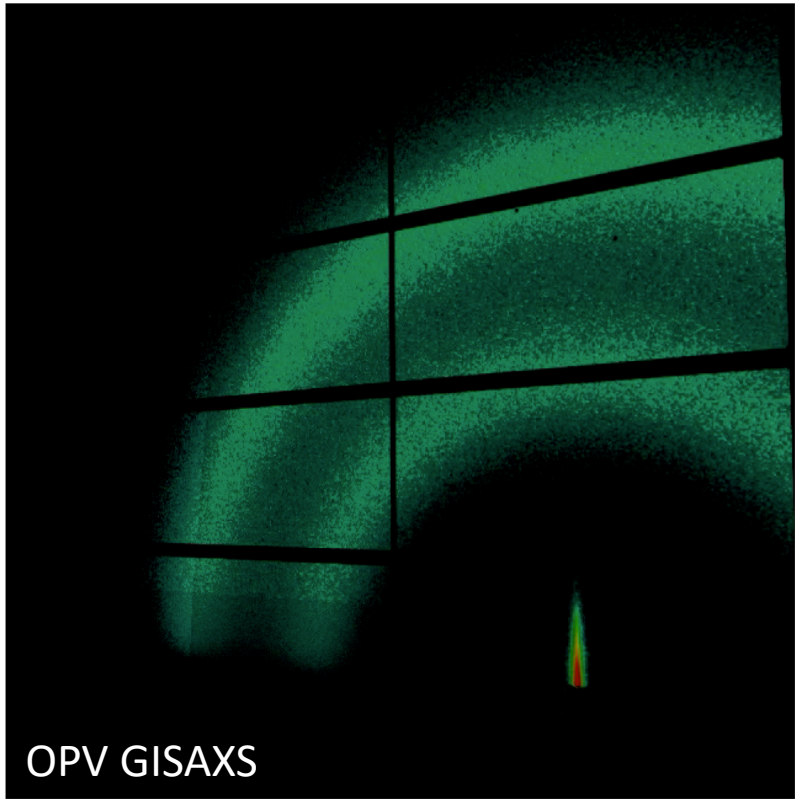
SENIOR STAFF SCIENTIST
PROGRAM LEAD FOR COMPUTING
ADVANCED LIGHT SOURCE
CENTER FOR ADVANCED MATHEMATICS FOR ENERGY RESEARCH APPLICATIONS

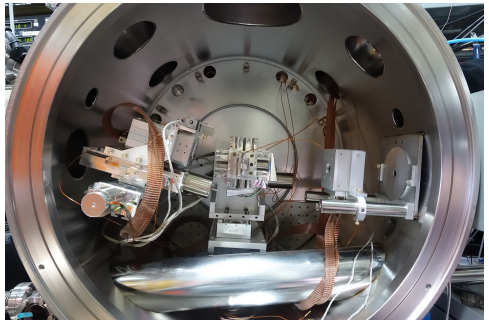
Fast and Complex Experiments at Light Sources

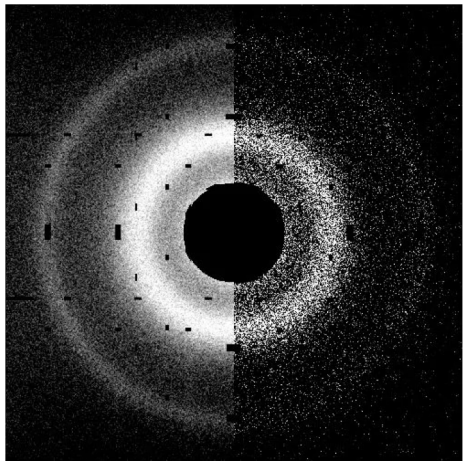


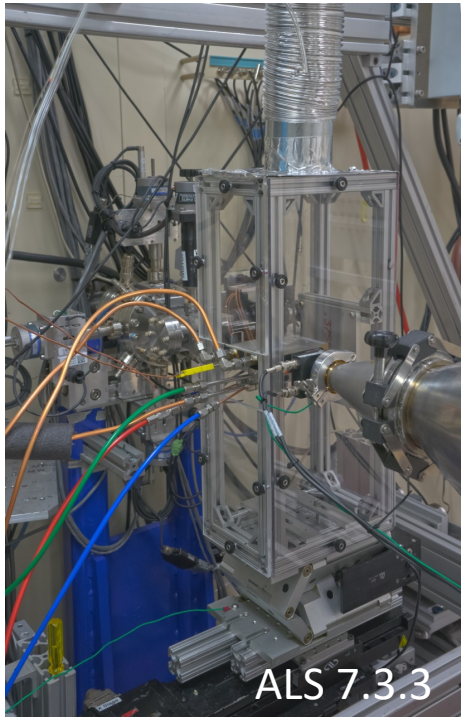


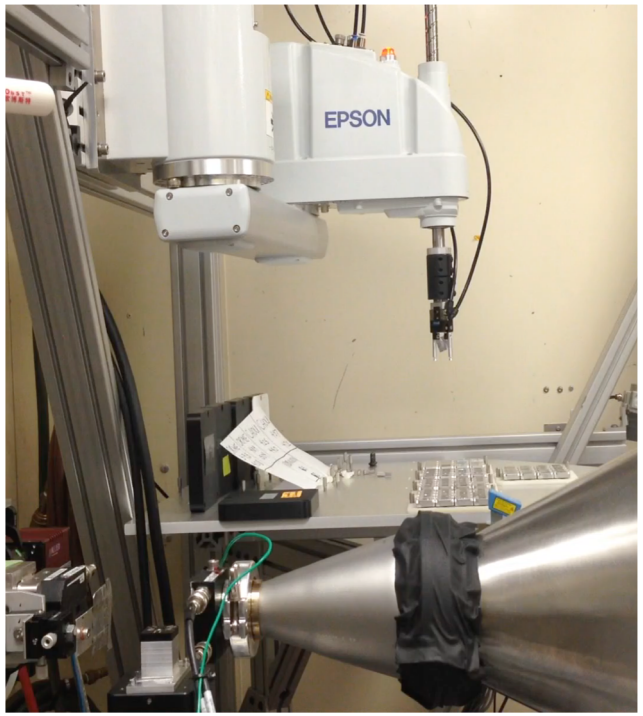


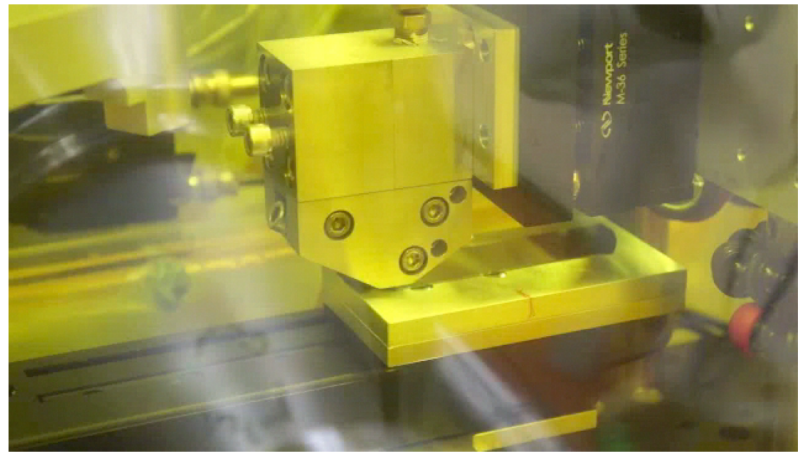






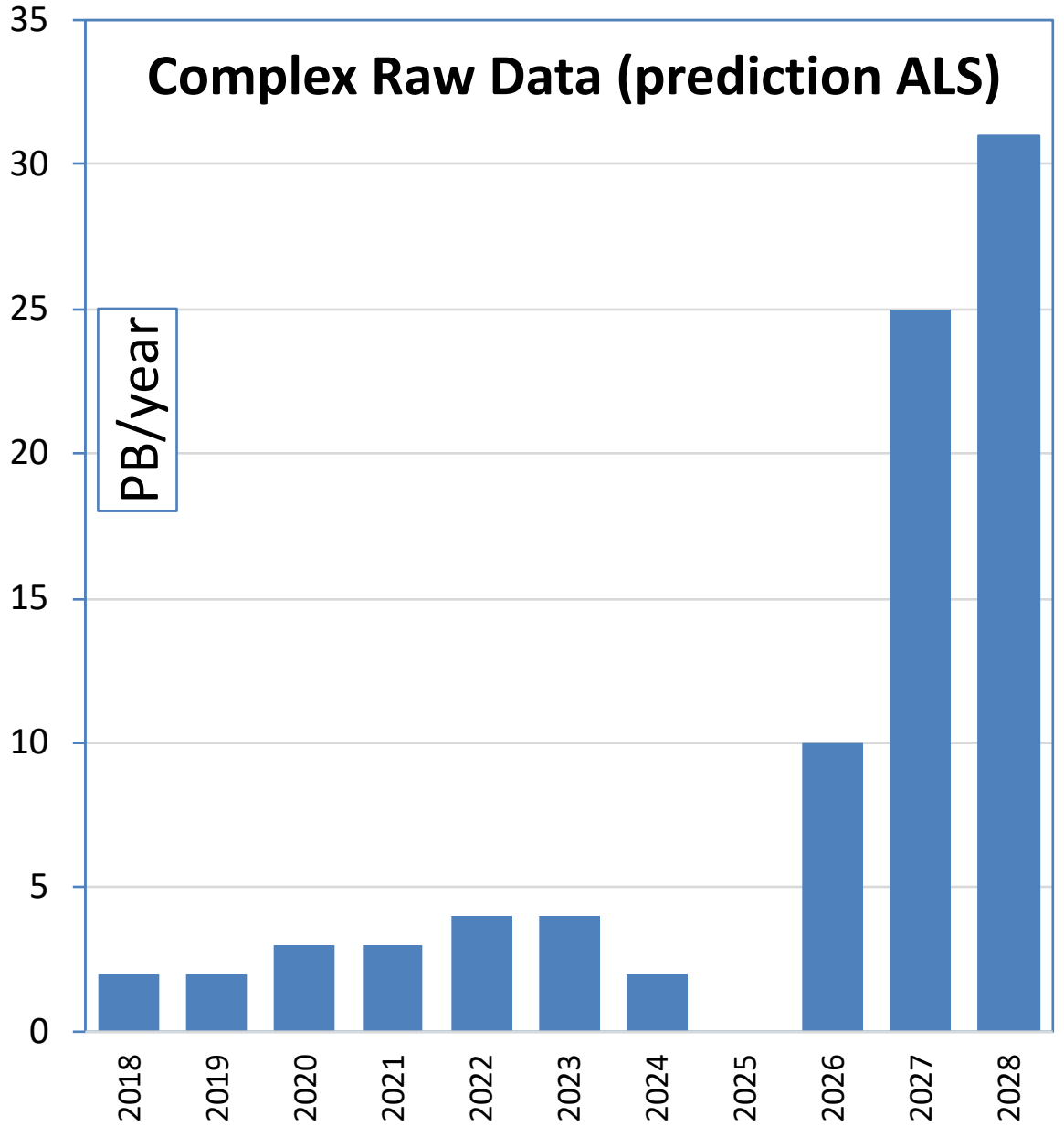


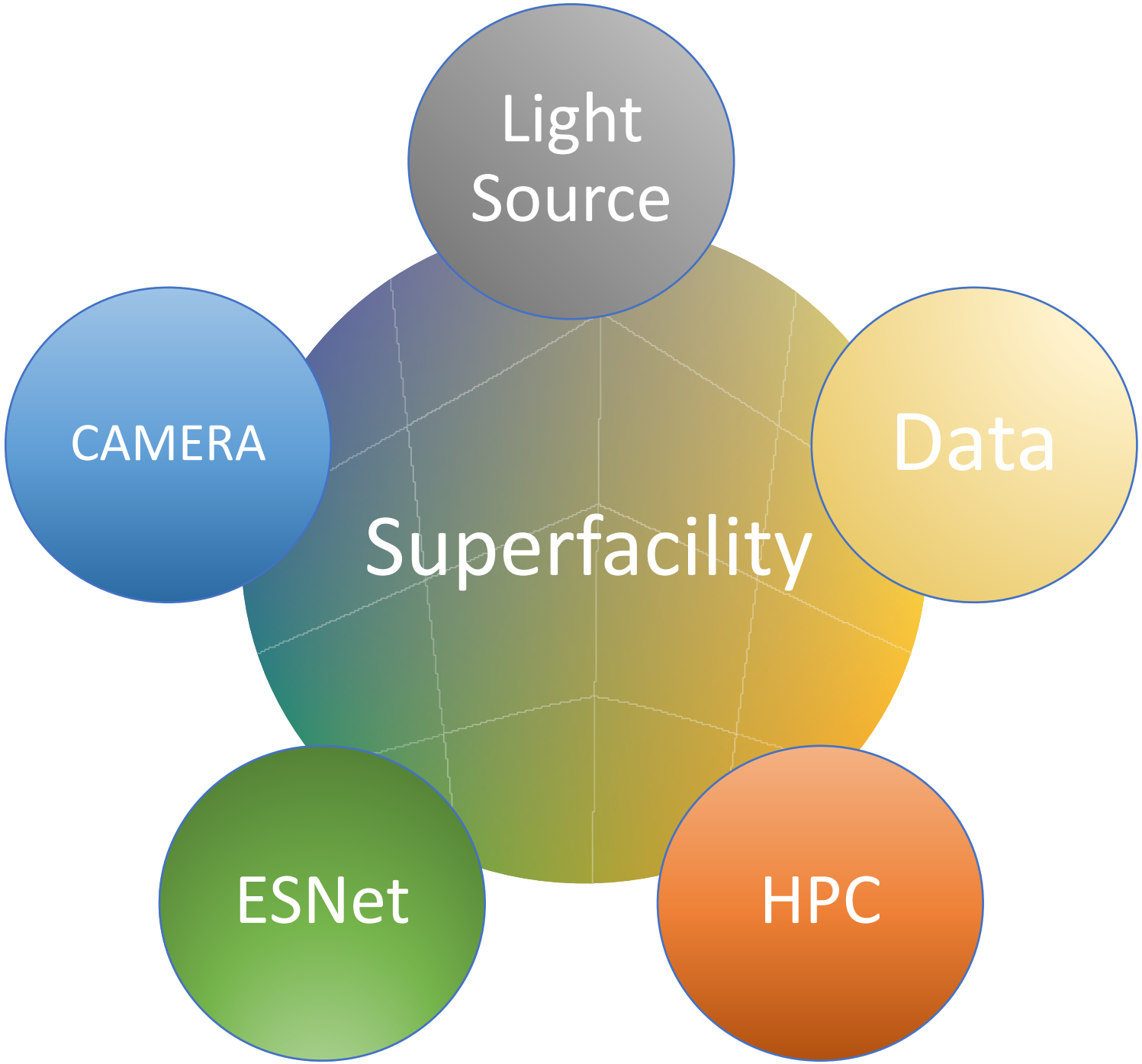




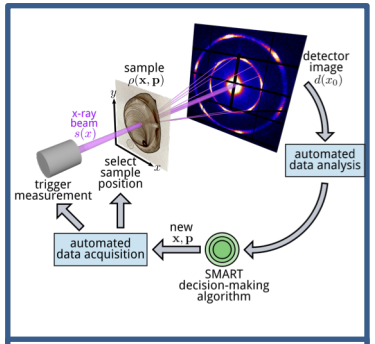
Challenges for User facilities

- >20% new users
- Provide very fast feedback and/or experiment combining data from different modalities
- Applying custom workflow to many data sets
- Need for new math and algorithms
- Make things easy and faster for users
- Data access across facilities
- Large amounts of data **or low counts**
- **DATA ANALYSIS WILL HAVE TO CHANGE**

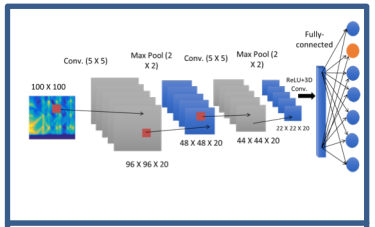



Light Source
CAMERA
Data
Superfacility
ESNet
HPC

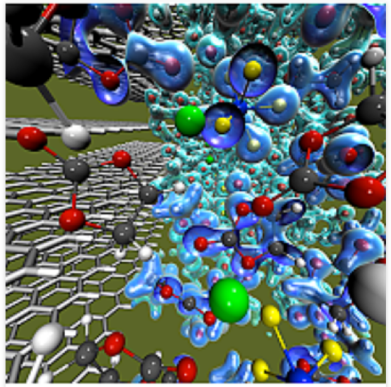
Center for Advanced Mathematics for Energy Research Applications



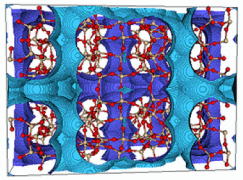
Autonomous Data Collection



Machine Learning

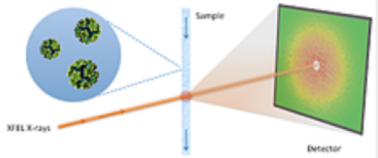


Electronic Structure

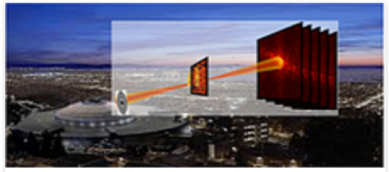


Material Informatics

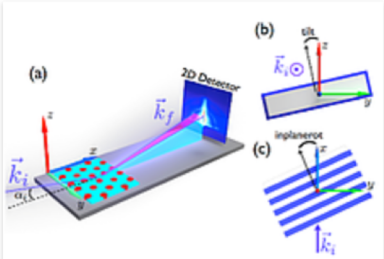
Nanocrystallography



Fluctuation Scattering



Ptychography



GISAXS

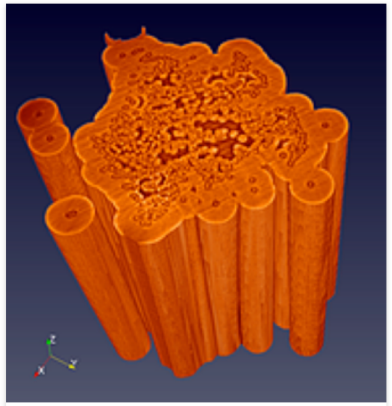


Image Analysis

Jamie Sethian
Head of CAMERA

DOE: BES and ASCR
Renewed last year

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

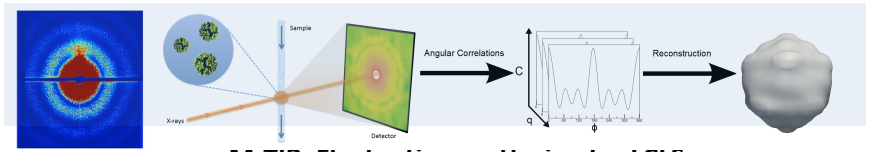
www.camera.lbl.gov

Overview of CAMERA Challenges:

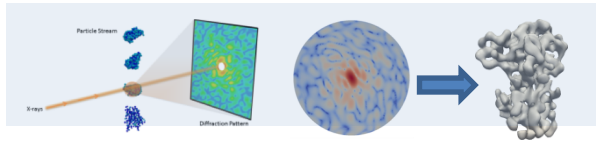
CAMERA Applied Math

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

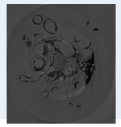
Goal: determine structure, function….



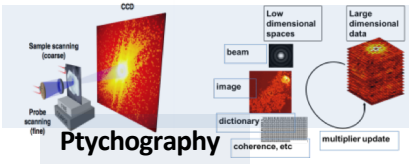
M-TIP: Fluctuation scattering for LCLS



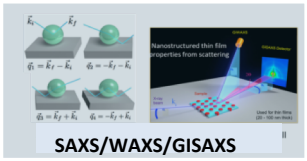
M-TIP: Single particle imaging for LCLS



TomoCAM: Fast GPU tomography for microCT



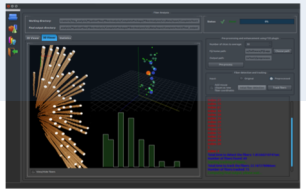
Ptychography



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

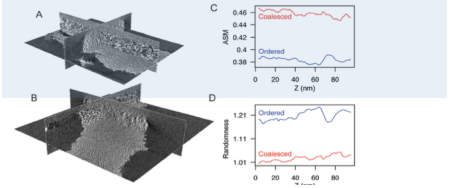
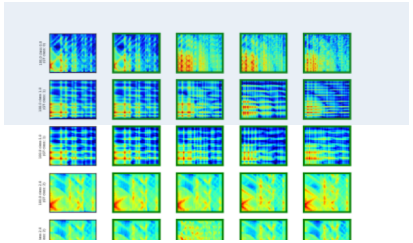
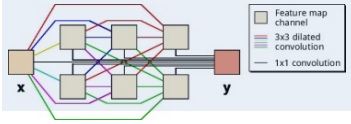
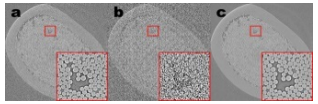


Image analysis for quality control during thin film manufacturing



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

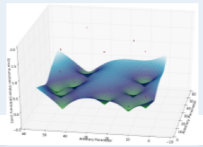




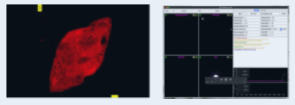
A new Mixed-Scale Dense Deep CNN for machine learning

How to use computing (embedded in detectors vs. local hardware/GPU vs. remote supercomputers) to quickly

Goal: Analyze/steer experiments as they happen



Autonomous Experiments



Nanosurveyor: Real-Time Streaming: ptychography

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

Goal: Working together

Xi-CAM: Platform for Synchrotron Data

In use at 13 beamlines across ALS, SSRL, NSLS II, APS, NIST . Free

CAMERA+ALS+SSRL+NSLSII

What is the scientific impact of all this?

CAMERA Applied Math

M-TIP for X-FEL fluctuation scattering
Multi-tiered iterative phasing reconstructs structure from X-FEL data at the LCLS.

Accelerating nanoporous materials discovery
Automatic, high-throughput mathematical characterization methods for EFRCs.

M-TIP for single particle imaging
Constrained projections for single particle imaging data at the LCLS

PEXSI for electronic structure
Fast methods to compute Kohn-Sham DFT theory for the Molecular Foundry and LLNL

GPU

Optimized autonomous experiments
Weighted Kriging algorithms to auto-steer experiments at NSLS-II and CFN (BNL)

TomoPy: Contributions to APS tomography package
Fast GPU-methods and NESAP NERSC postdocs, joint with APS.

GPU

GPU

Ptychographic reconstruction: SHARP
Scalable Heterogeneous Adaptive Real-Time Ptychography (ALS, SSRL, and LANL)

TomoCAM: Fast reconstruction for micro-CT
Non-uniform FFTs for faster reconstruction for MBIR APS (TomoPY) and ALS

GPU

GPU

Machine Learning for biological and materials images
Mixed-Scale Dense CNNs for automatic image analysis and tomography at ALS and CWI

Real-time streaming of synchrotron data
Real-time streaming end-to-end environment for immediate, automatic data analysis at ALS

GPU

X-ray Scattering Algorithms
Fast GPU-methods for CD-SAXS CD-GISAXS for APS, NIST, and the ALS

Xi-CAM: Community platform for synchrotron analysis
GUI, applications plug-in and remote workflow: NSLS-II, SSRL, ESRF, APS, LCLS, NIST, DESY, ALS.

GPU

GPU

Structure recognition for ceramic matrix composites
Automatic structure identification and machine learning for scattering, for GE, ALS and NCEM

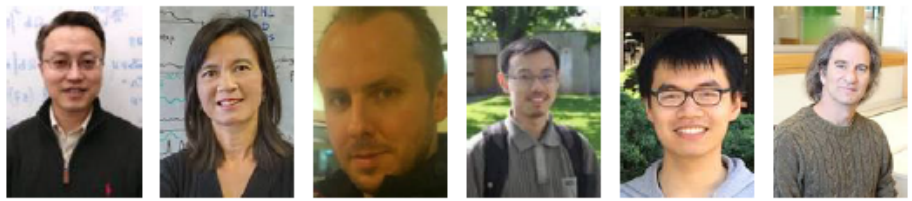
Community workshops and summer schools
Workshops= Tomography, Image Analysis
Summer schools= Electronic structure, GISAXS

CAMERA Members

J.J. Donatelli (A,B) | P.H. Zwart (A,B) | K. Pande (A,B) | D. Ushizima (C,G,I,L) | M. Macneil (C,G,I,L) | T. Perciano (C) | S. Marchesini (D,E)

D. Shapiro (D) | P. Enfadeque (D) | H. Chang (D) | D. Parkinson (E,F) | A. Hexemer (F,G,H) | R. Pandolfi (F,G,H) | M. Noack (M)

D. Kumar (E,F,G) | G. Freychet (H,M) | D. Pelt (C,E,J) | O. Jain (I) | S. Mo (I) | H. Krishnan (C,D,E,F,G) | L. Lin (J)



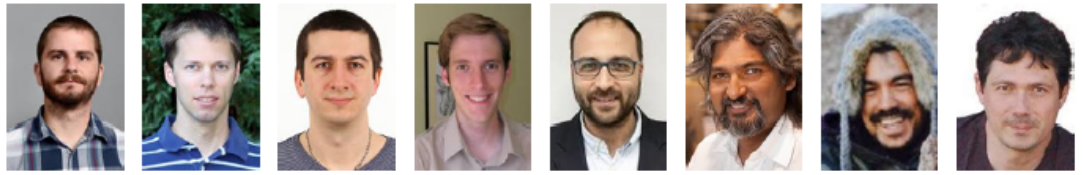
C. Yang (J) | X. Li (J) | M. Haranczyk (K) | M. Shao (B) | Z. Hu (A) | J.A. Sethian

A=Fluctuation scattering/Single particle, B=Exafel, C=Image Analysis, D=Ptychography/streaming, E=Tomography, F=Xi-CAM, G=GPU/Hardware acceleration, H=Scattering, I=Machine learning, J=Electronic Structure, K=Chemical Informatics, L=BioInformatics, M=Optimization

CAMERA Collaborators

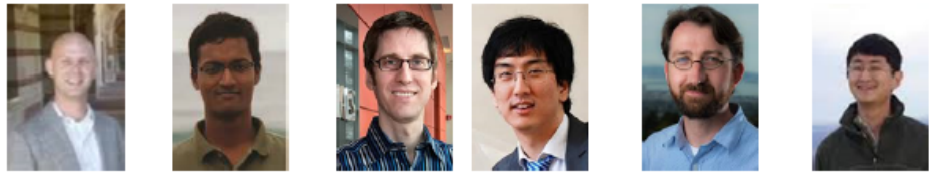
D. Allan (BNL) | A. Aquila (SLAC) | T. Caswell (BNL) | K. Champley (LLNL) | B. Daurer (Uppsala) | F. DeCarlo (APS) | E. Dill (BNL) | L. Fourcar (Max Planck)

M. Fukuto (BNL) | C. Gati (SLAC) | C. Gheller (CSCS) | A. Gorel (Max Planck) | M. Grunbein (Max Planck) | D. Gursoy (APS) | E. Herzig (Bayreuth) | M. Hunter (SLAC)



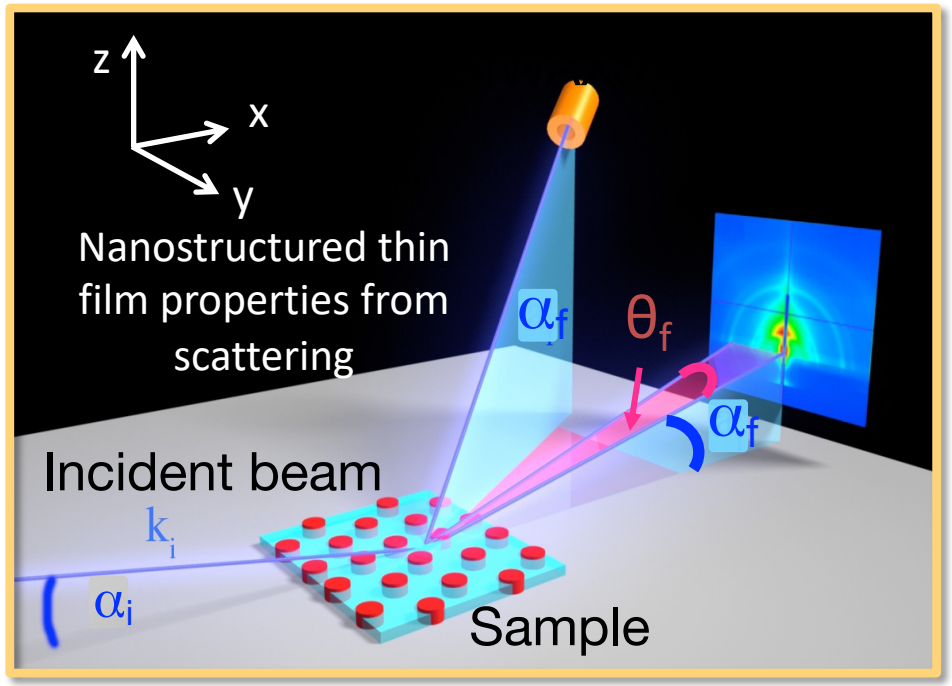
R. Kirian (Arizona) | J. Klein (NIST) | R. Kurta (E-XFEL) | F. Maia (Uppsala) | A. Mancuso (E-XFEL) | A. Mehta (SSRL) | D. Mendez (Arizona) | A. Perazzo (LCLS)

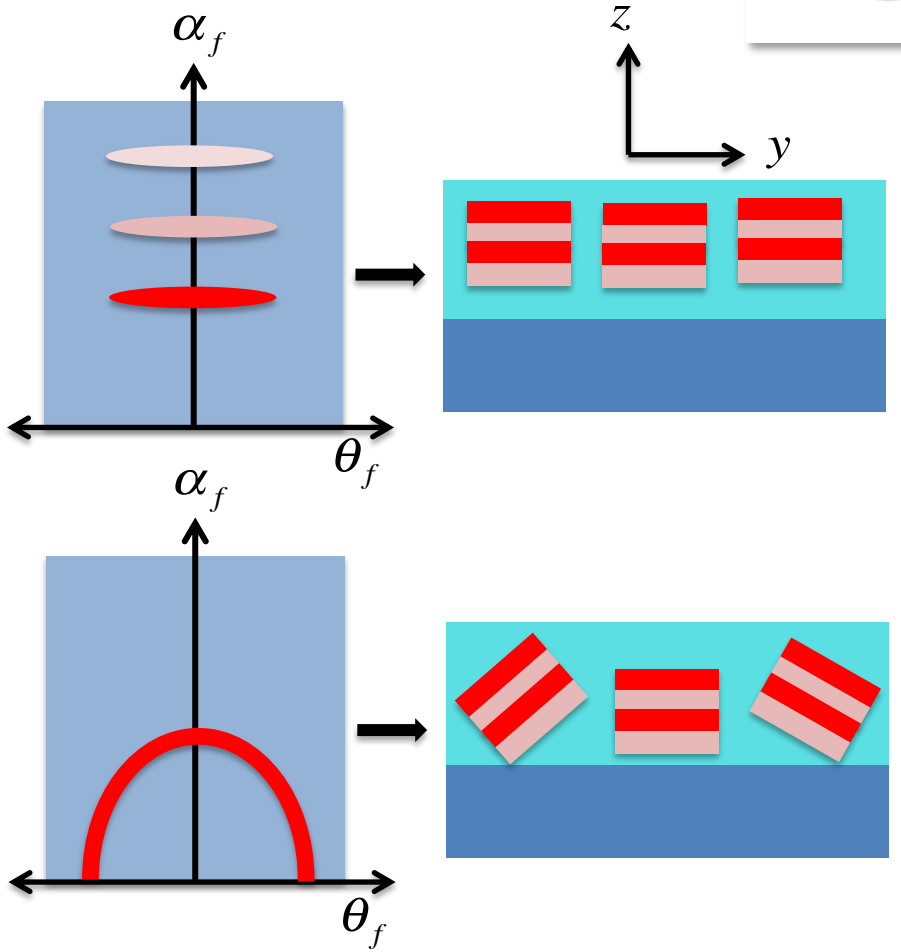
.. Pellouchoud (SSRL) | L. Richter (NIST) | A. Sakdinawat (SLAC) | I. Schlichting (Max Planck) | A. Sepe (SSRF) | R. Sierra (SLAC) | J. Strzalka (APS) | C. Sweeney (LANL)



C. Tassone (SSRL) | S. Venkatakrishnan (ORNL) | K. Yager (BNL) | C. Yoon (SLAC) | D. Prendergast (Molecular Foundry) | J. Zhang (APS)

GISAXS

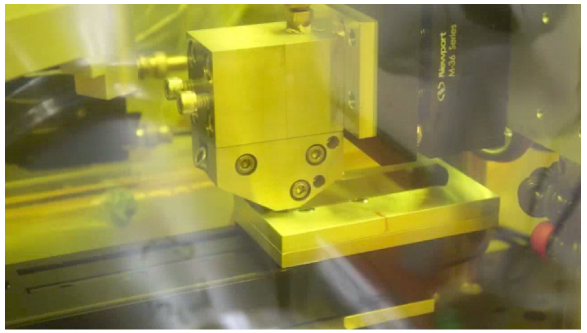


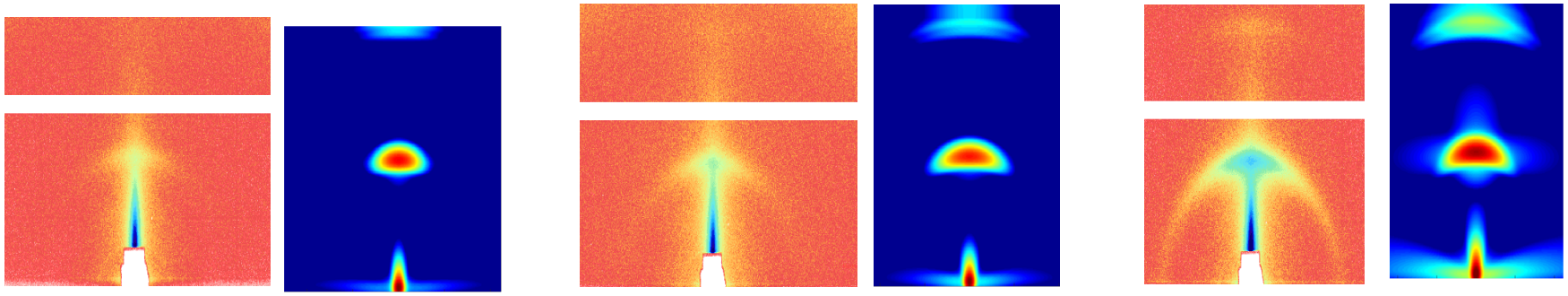


Applications : photo-voltaic, liquid crystals etc.

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

Real-time Interaction with HPC





2014

- 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

Deployment of Mathematical Algorithms: Xi-cam

Scientific Achievement

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

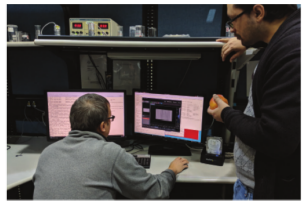
Research Details

- Remote processing with HPC for real-time high data rate analysis
- remote data access for high-volume data retrieval
- Highly interactive design

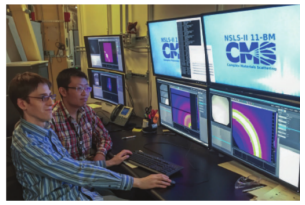
APS: 2-BM, 8-ID-E
BNL: 11-BM, 6-BM, 12-ID
SSRL: 2-1, 1-5
ALS: 7.3.3, 5.3.1, 11.0.1.2, 6.3.1.2, 8.3.2
NIST CDSAXS Group
Universities: Fribourg, Berkeley, Colorado, Kent State, TU Munich, Penn State, UC Davis
Industry: DOW, Rivera, GE

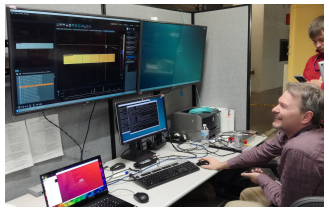
Xi-CAM plug-ins

Tomography
Time resolved SAXS
Electron Microscopy
NEXAFS
iPython
Globus Online
Databroker
Remote Computing
GISAXS
HIPGISAXS
GIWAXS simulator
Reverse Monte Carlo
CD-GISAXS
Plug-in Store


APS 2-BM


APS 8-ID-E

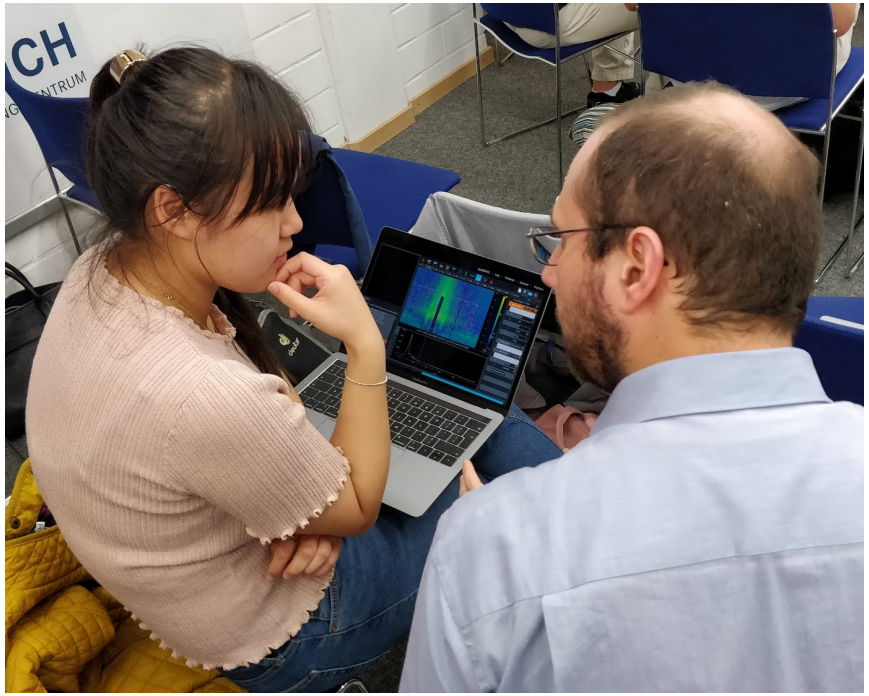

BNL 11-BM


BNL SMI Beamline

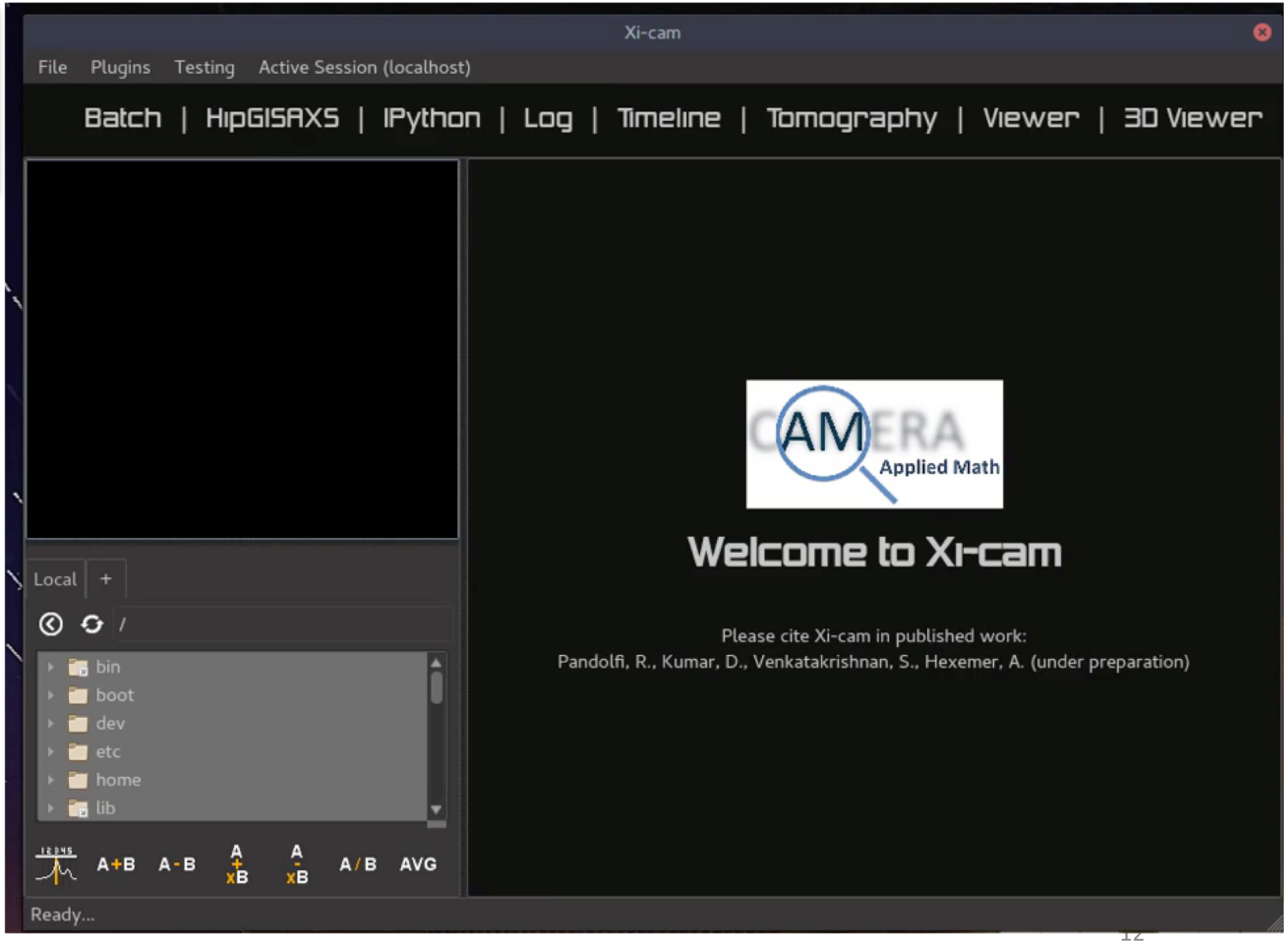
Remote Execution

UNIVERSITÄT BAYREUTH

GISAS Summer School 2018

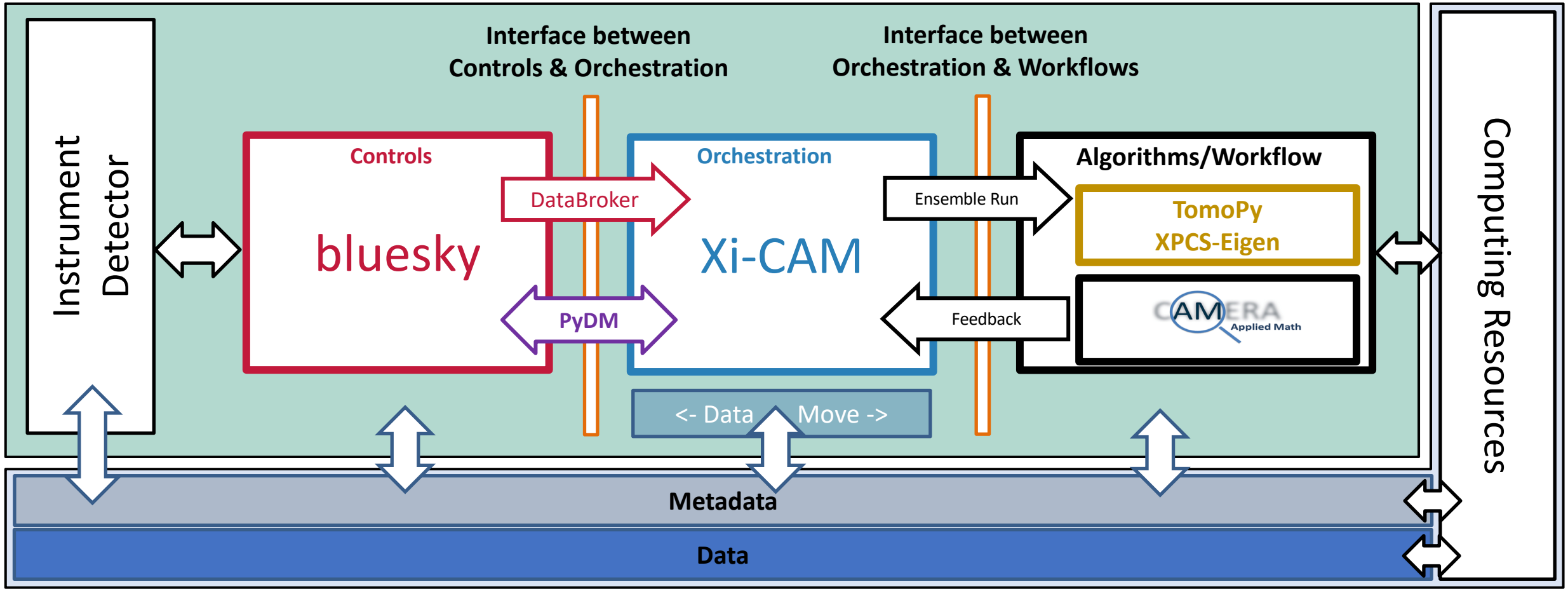


GISAXS Workshop in Bayreuth in collaboration with CAMERA

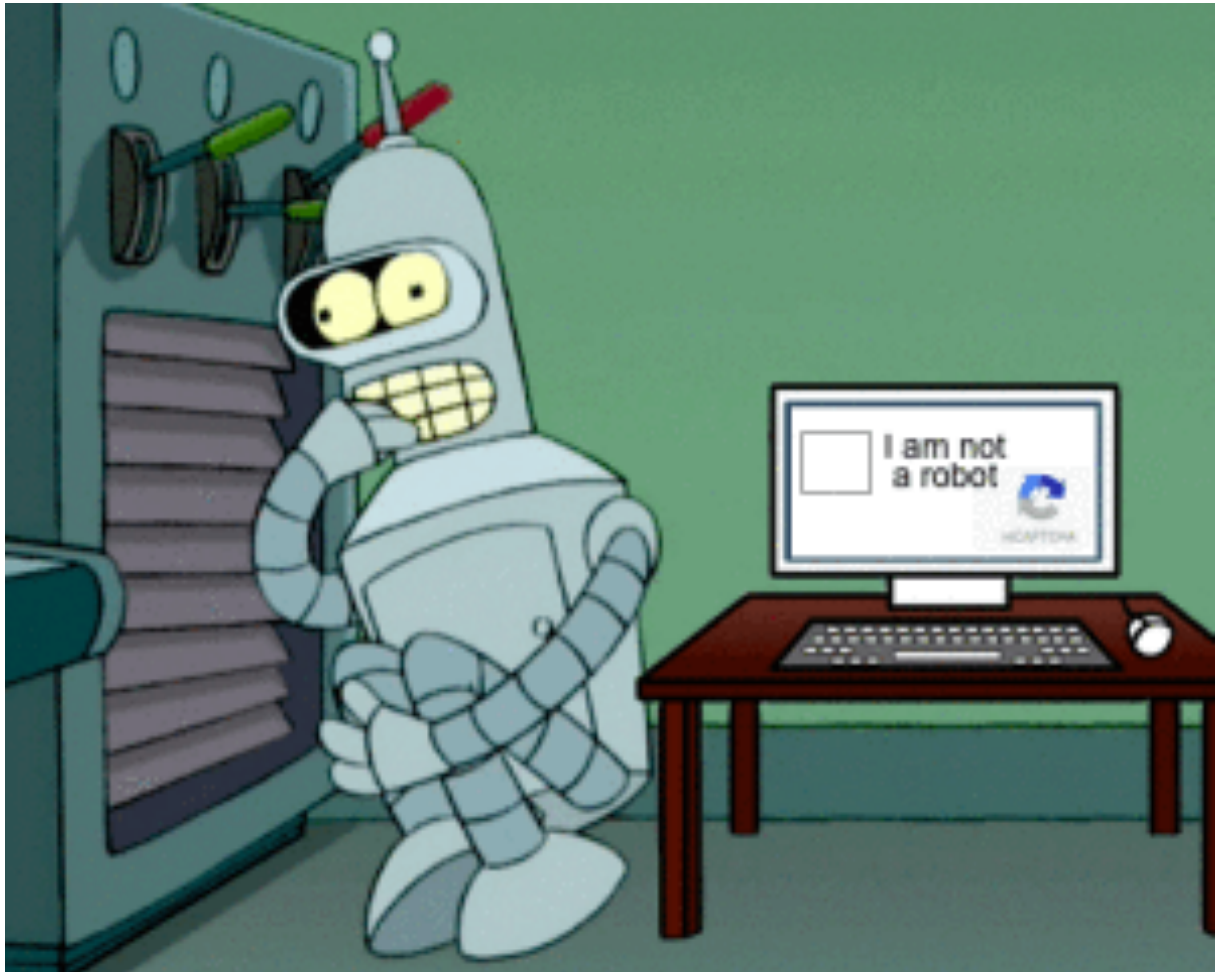


BES Data Task Force Pilot (2 years)

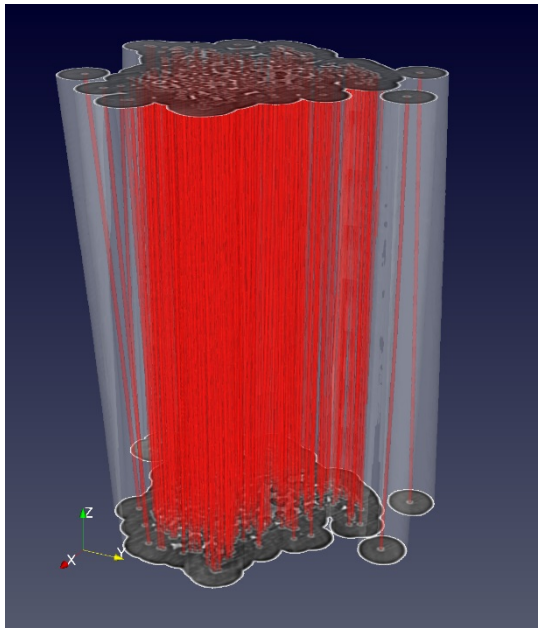
Alexander Hexemer ALS, Nicholas Schwarz APS, Amedeo Perazzo LCLS,
Stuart Campbell NSLS II, Apurva MehtaSSRL



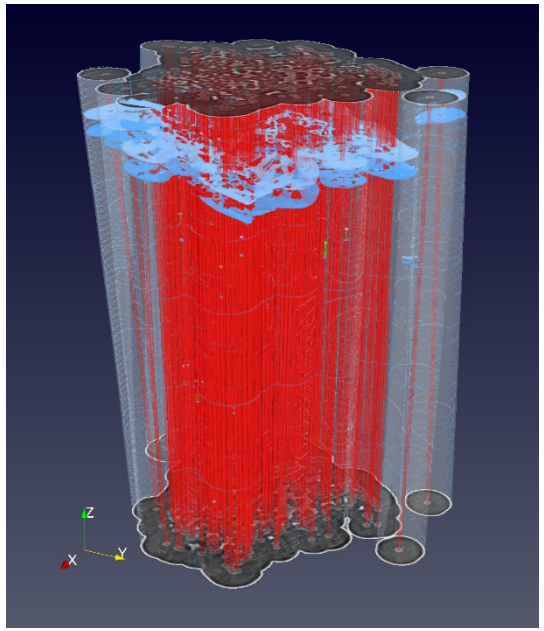
Machine Learning



Fibers, fiber breaks, and cracks

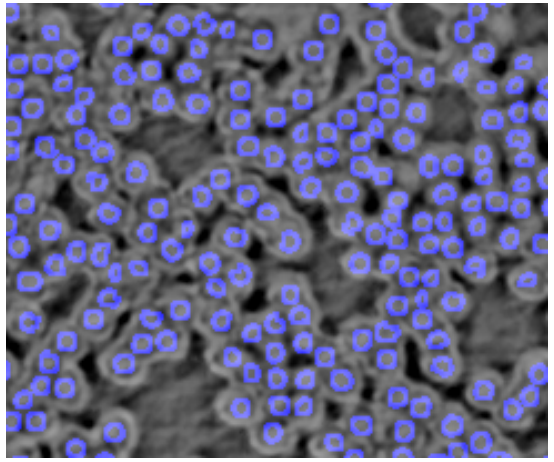


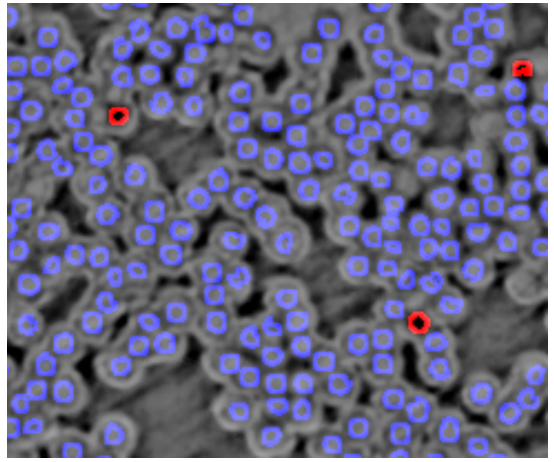
93N



151N

Slice #

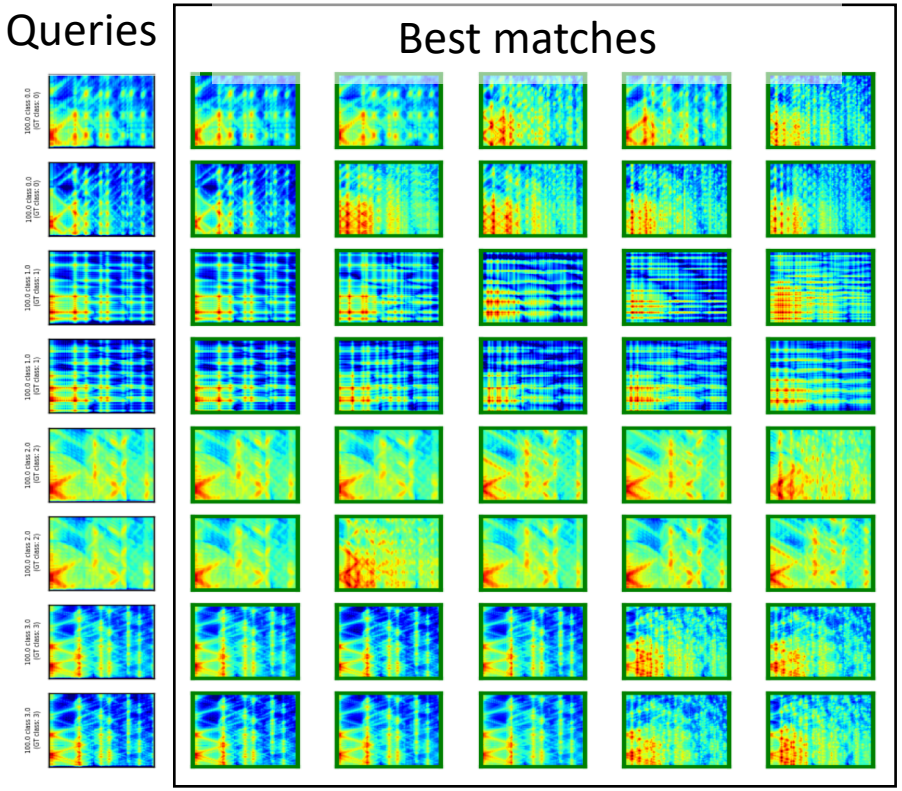


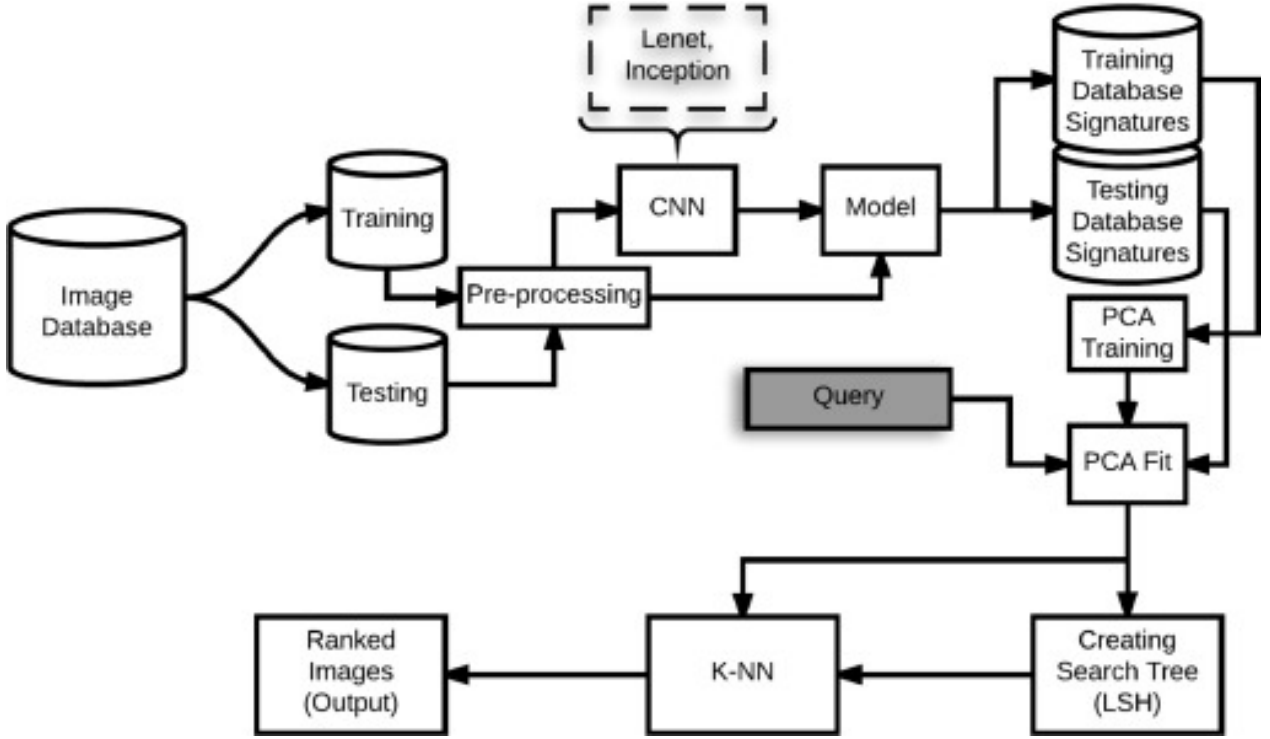


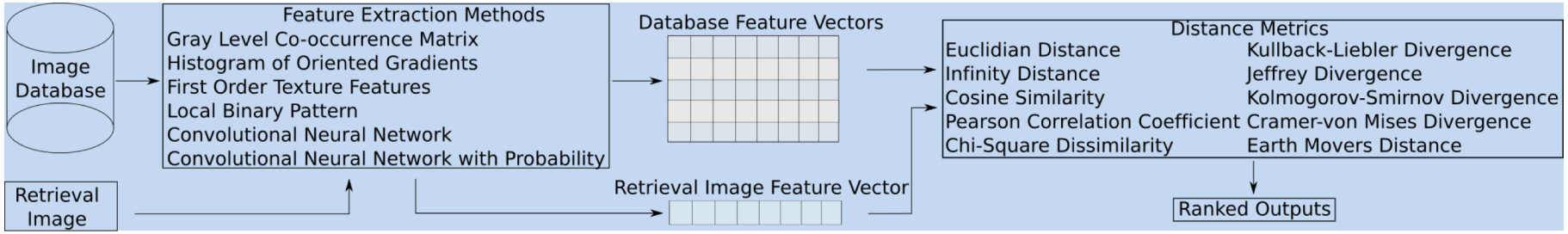
D. Ushizima, T. Perciano, H. Krishnan, B. Loring, B. Hrish, D. Parkinson, R. Ritchie, W. Bethel and J. Sethian,

Rick Perry Explores GE CMCs
Spring 2018

Deep Learning for X-ray Diffraction

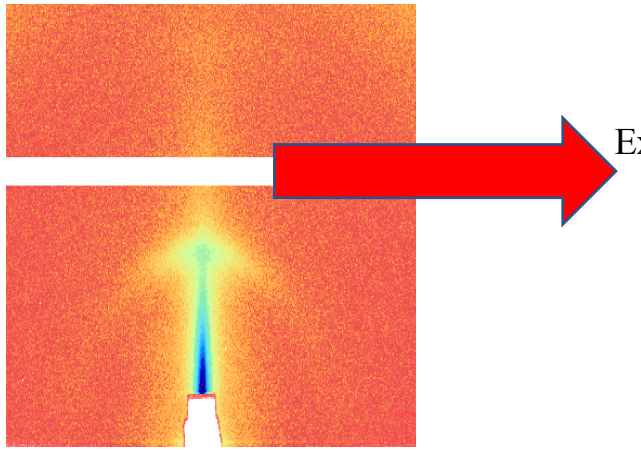






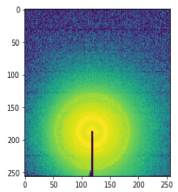
Expert Systems with Applications: Volume 109, 1 November 2018, Pages 35-48
Reverse image search for scientific data within and beyond the visible spectrum: Flavio H.D. Araujo, Romuere R.V.Silva, Fatima N.S. Medeiros, Dilworth D. Parkinson, Alexander Hexemer, Claudia M. Carneiro, Daniela M. Ushizima

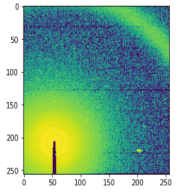
ML for Online Scattering Analysis



Experiment Images

SAXS/WAXS → Integration as a function of radius

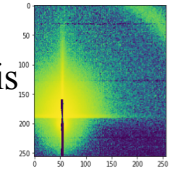




GISAXS/GIWAXS

Stage 1: Finished
>95% accuracy

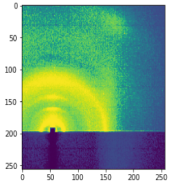
Featureless → No further analysis/manual analysis



Features

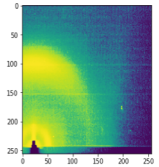
Rings

Full rings



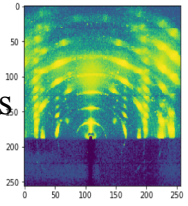
Linecut/Integration as a function of radius

Arcs

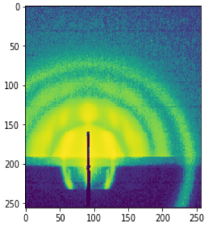


Peaks → Convolutional Neural Networks

Simulation >98% accuracy
Experiment >70% accuracy



Rods → Linecut/Integration over qz

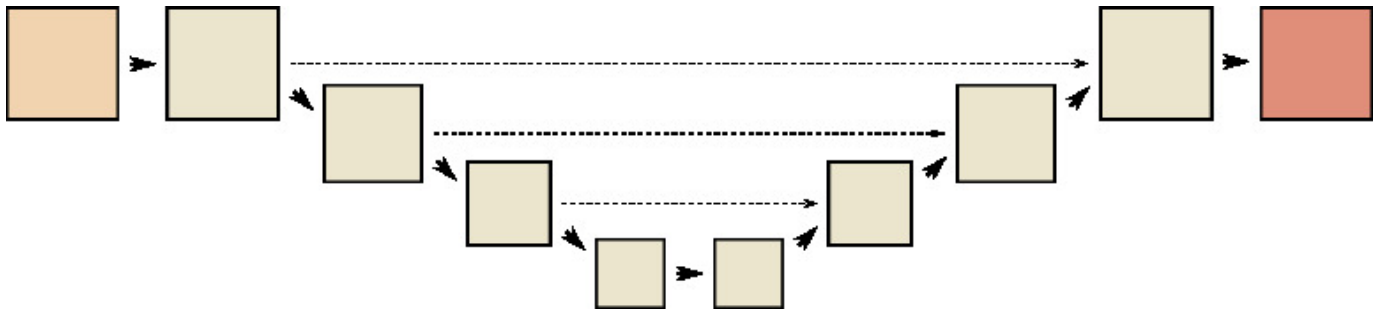


Stage 2: Optimizing
>90% accuracy

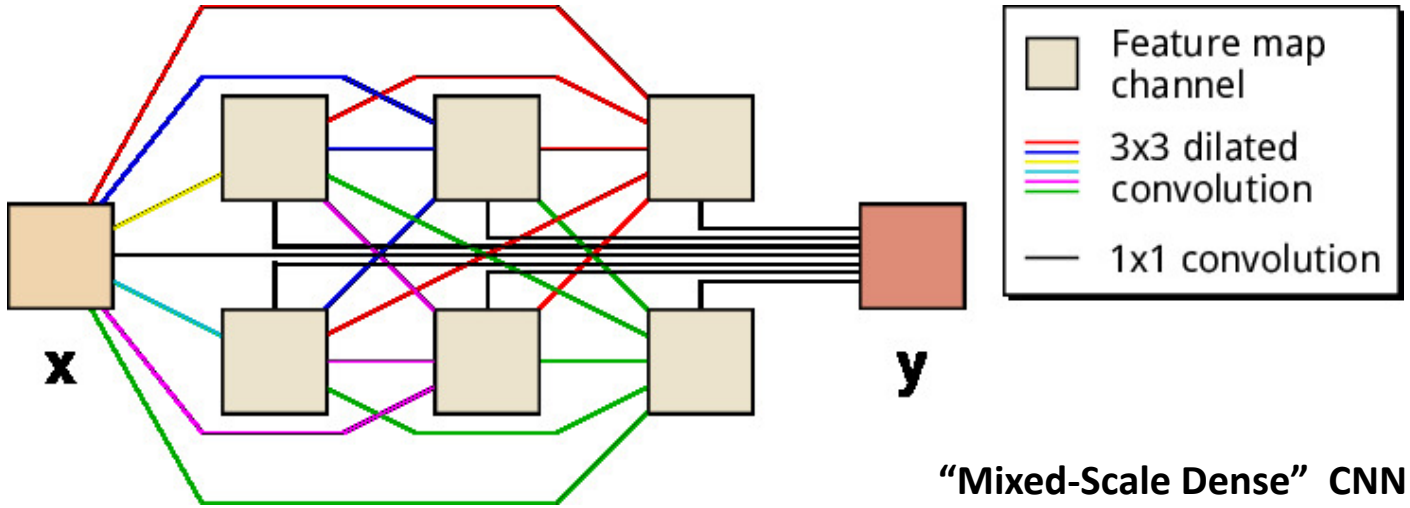
Stage 3: Exploring
>80% accuracy

Mixed-Scale Dense Convolution Neural Network (MSD)

- Standard Deep CNN's (Caffe, TensorFlow, VGG, AlexNet…)
  - Multiple layers
  - Down- and up-sampling
  - Millions of parameters to train
- Mixed-scale dense CN
  - Replace down- and up-sampling with dilated convolutions
  - Densely connect all feature maps
  - Far fewer parameters to train, less chance of sticking in local minima
  - Robust—same parameters for different applications



Standard Deep CNN



"Mixed-Scale Dense" CNN

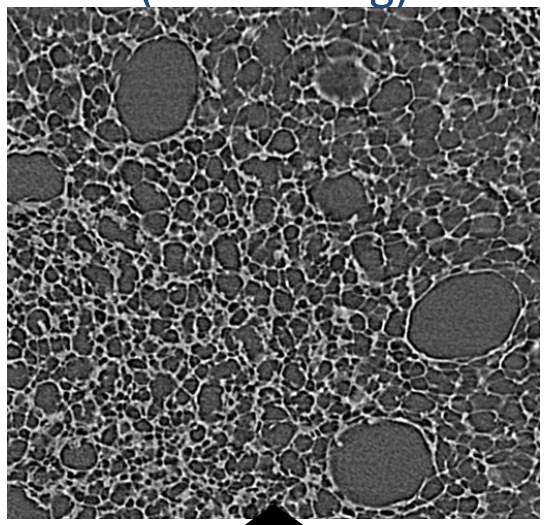
Pelt and Sethian, A Mixed-Scale dense convolution neural network for image analysis, PNAS (2018) v115n2, p254

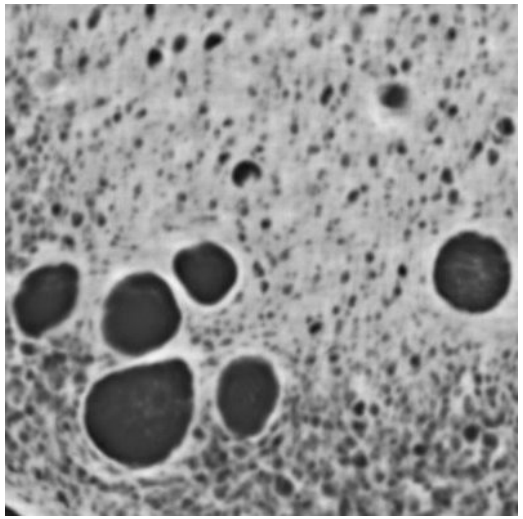
Training

Static scan
(for training)

Time-resolved
scan

1024 angles
(original)

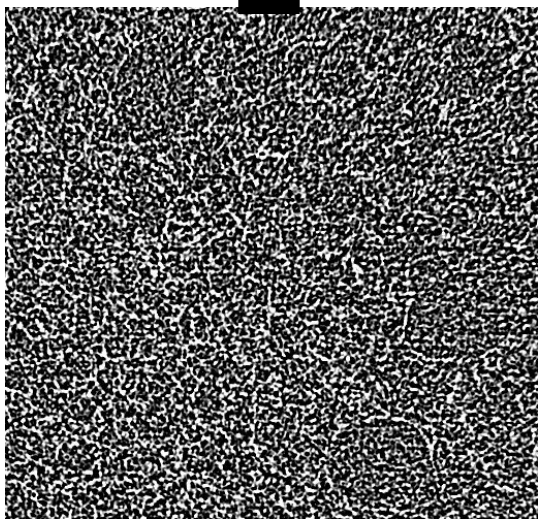


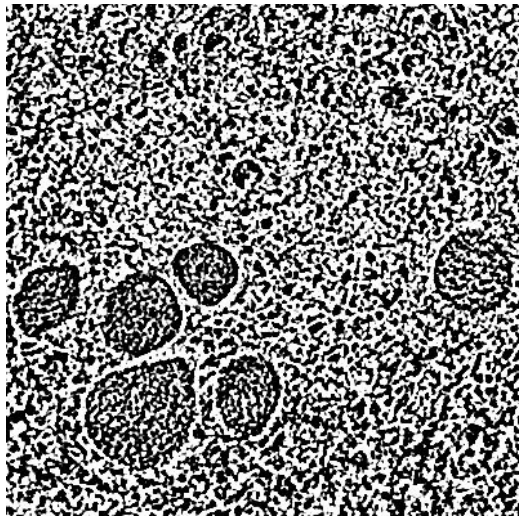


Output of
Mixed-Scale
Dense Network

Train

128 angles
(downsampled)





Standard
Reconstruction
of128 angles

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