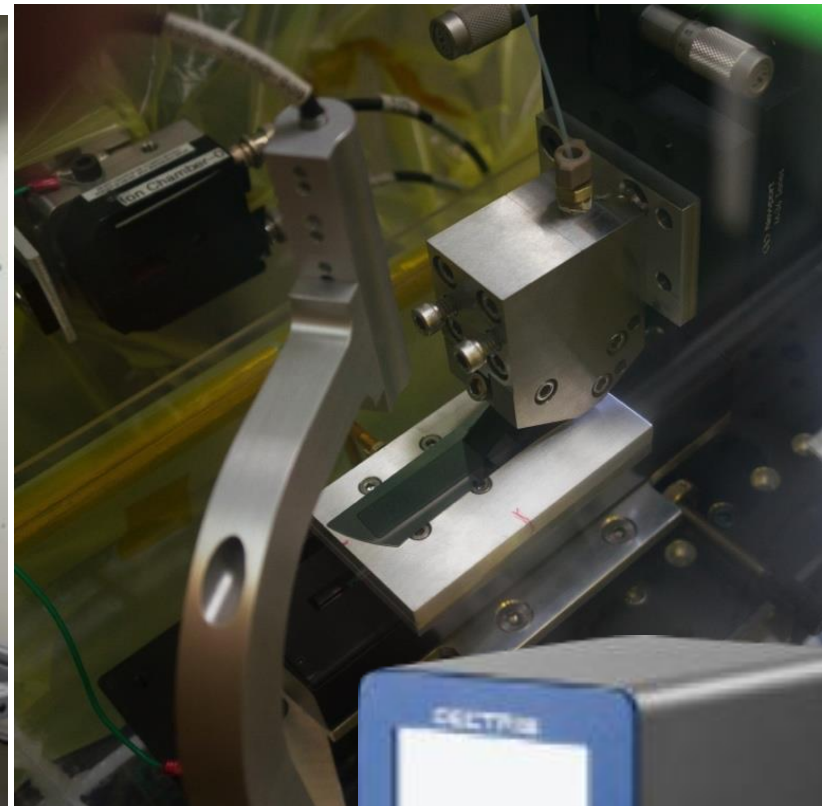
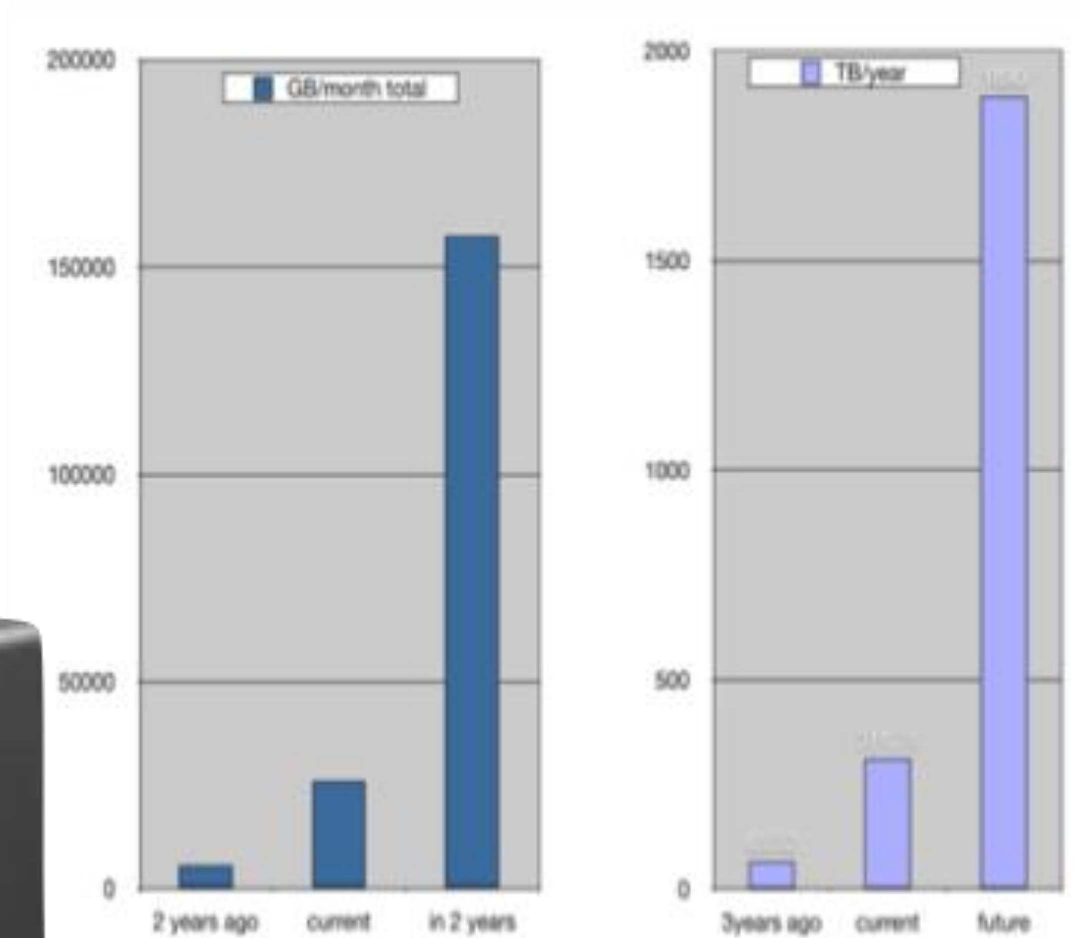
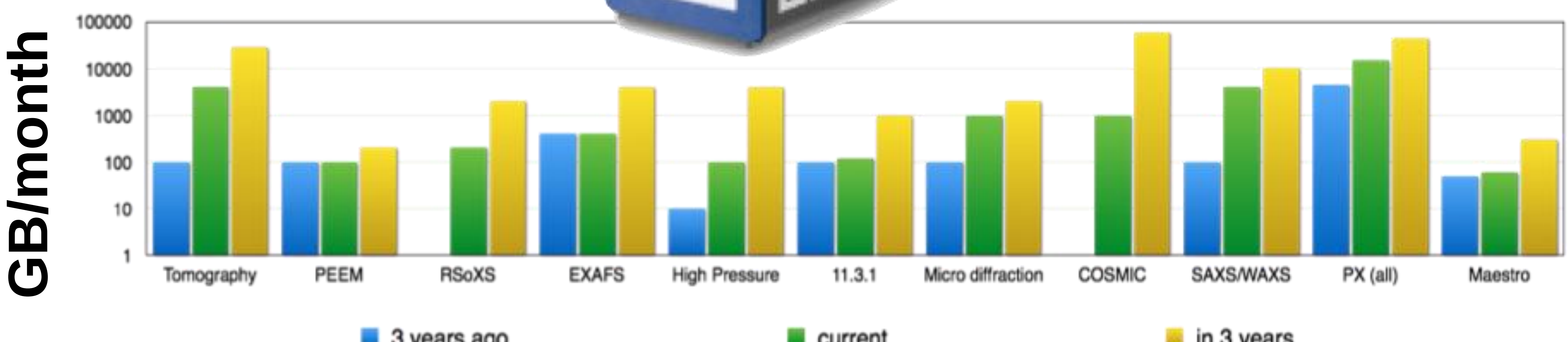
Data Challenge

up to 2 Petabytes /year of raw data.

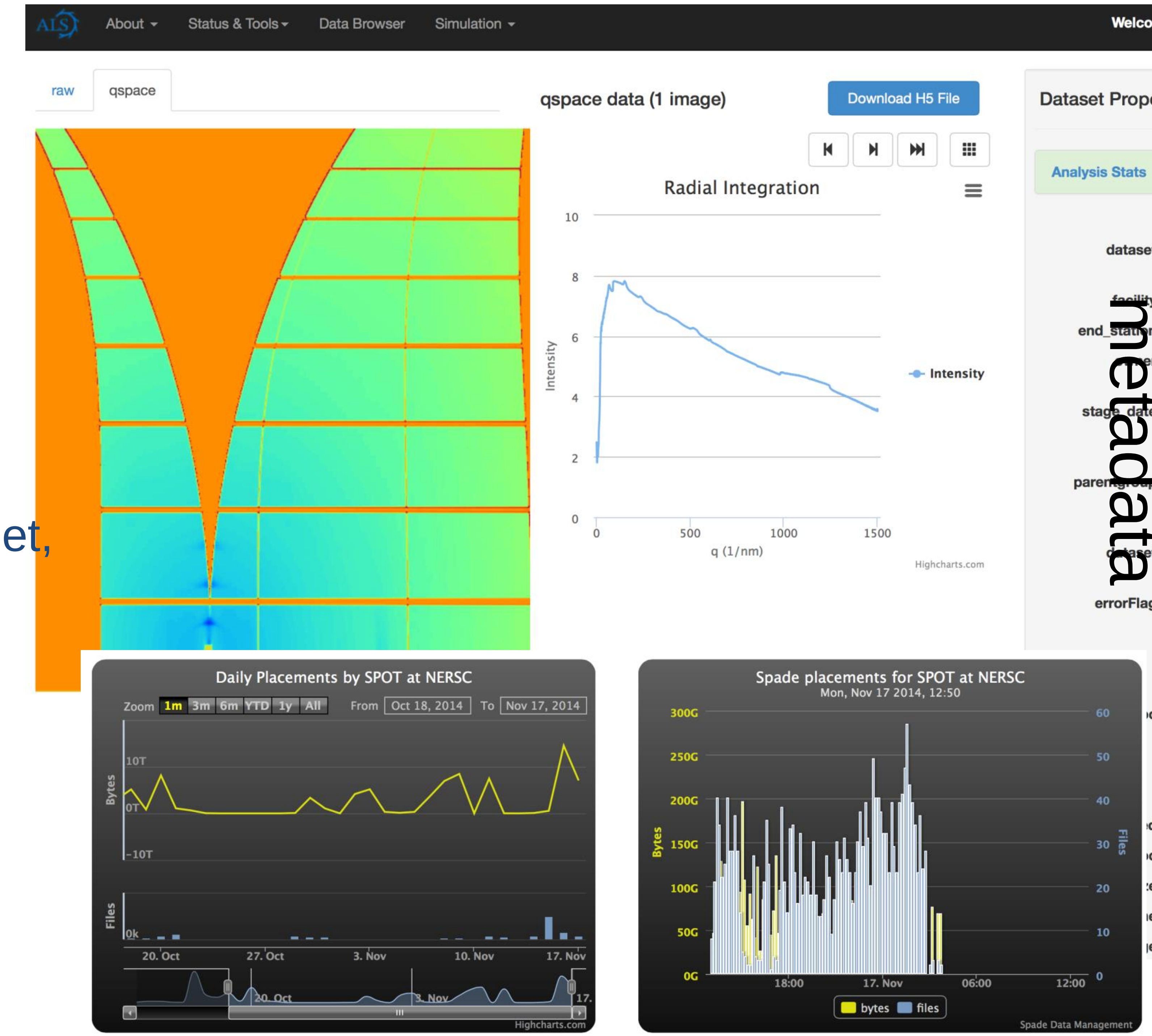




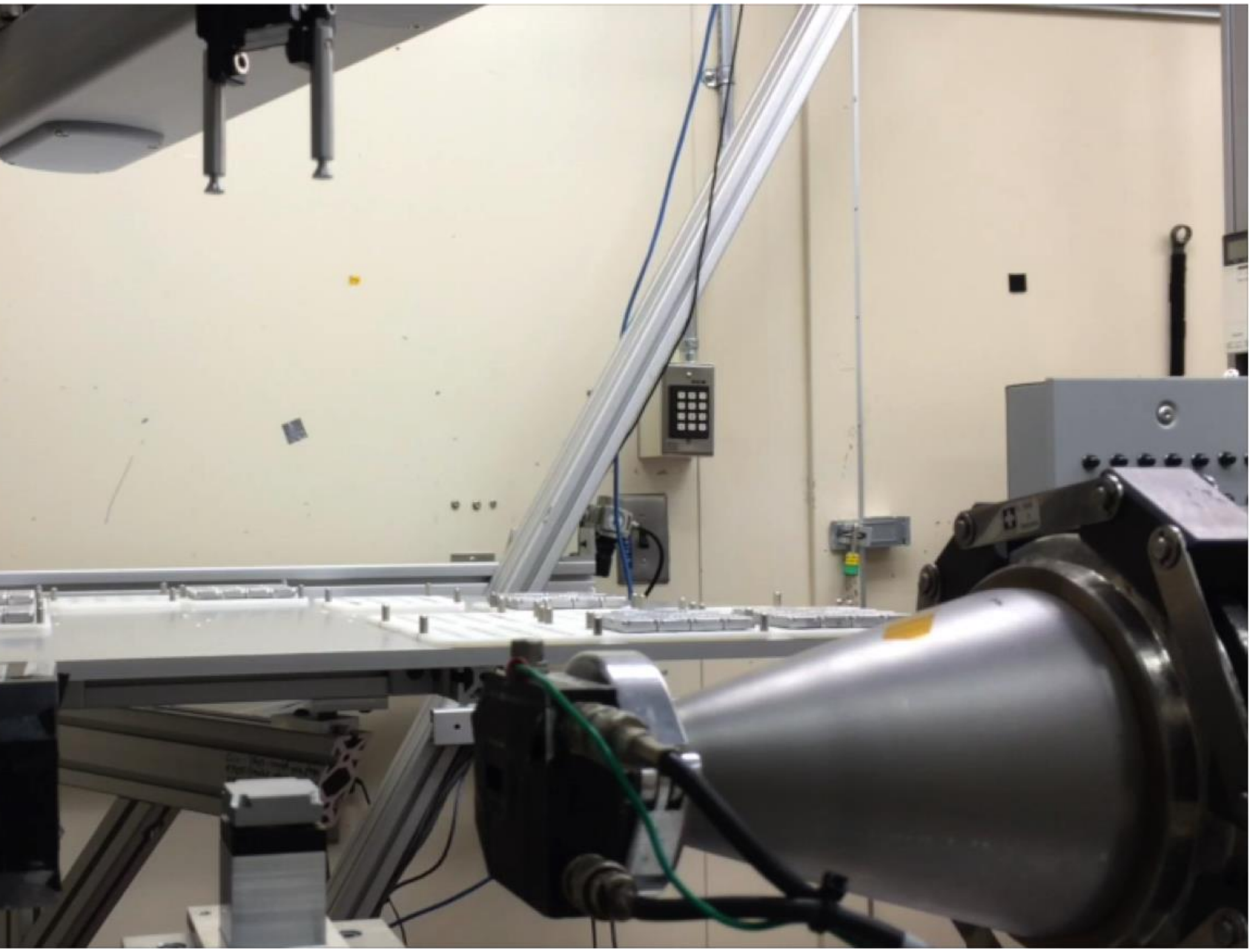


LBNL SPOT Suite: Towards an End-to-End Solution for Light Source Data, Analysis, & Simulation

- ALS generates Big Data.
- Scientists need accessible…
  - scalable software systems.
  - HPC/HTC/network resources.
  - advanced algorithms & analysis.
  - advanced simulation.
  - realtime feedback.
  - remote visualization
- Multi-division team: CRD, ALS, ESNet, MSD, & NERSC.
  - LDRD & BES/ASCR data pilots
- Focus on in-situ, time-resolved experiments, new algorithms, data sharing & collaboration.



Remote experiments now a reality.



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”

HIPGISAXS (now part of CAMERA)

CAMERA: Center for Applied Mathematics for Energy Research Applications

earch Applications (CAMERA) is an integrated, cross disciplinary center aimed at inventing, developing, and delivering the fundamental new mathematics required to capitalize on

CAMERA

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- About
- Background and Talks
- Location
- Members
  - Alumni
- News
- Projects
  - Electronic Structure
  - GISAXS
    - GISAXS: Current and Future Work
    - GISAXS: Examples
  - Image-based experiments
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- Publications
- Software
  - HipGISAXS
  - PEXSI
  - Sharp_Camera_...
  - Zeo++
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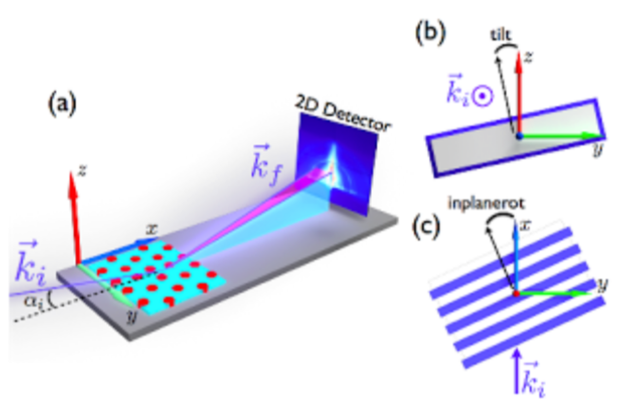
- Workshops and Tutorials
  - SHARP workshop, LBNL Oct 8

Project: GISAXS

X.S. Li, A. Hexemer, S. Chourou, A. Sarje

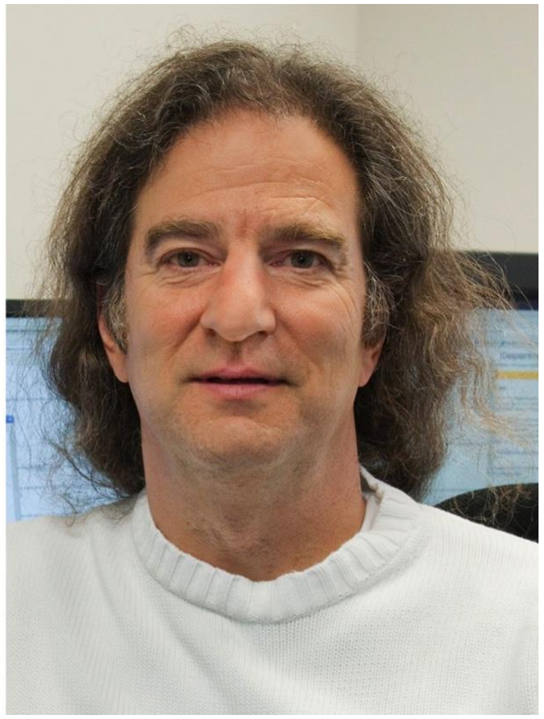
Faster Analysis for X-ray Scattering Data



Grazing Incidence Small Angle X-ray Scattering (GISAXS) is a unique method for characterizing the nanostructural features of materials, particularly at surfaces and interfaces, which would otherwise be impossible using traditional transmission-based scattering techniques. It is a surface-sensitive tool for simultaneously probing the electron density of the sample both in-plane and out-of-plane, and is being increasingly utilized to measure the size, shape, and spatial organization of nanoscale objects located on top of surfaces or embedded in mono- or multi-layered thin film materials. Individual GISAXS images serve as static snapshots of nanoscale structure, while successive images provide a means to monitor and probe dynamical processes, including self-assembly or other reorganization events, which occur at nanometer length scales. The success of GISAXS relies on the unique information that can be extracted from the data. Although microscopy techniques provide very valuable local information on the structure, GISAXS is the only one to provide statistical information on nanometer features averaged over large centimeter sample sizes. Presently a major bottleneck preventing GISAXS from reaching its full potential persists in the availability of data analysis and modeling resources for interpreting the data.

Examples | Current and Future Work | Publications

CAMERA



Jamie Sethian
Head of CAMERA

Printing Organic Photovoltaics & Realtime Analysis

- **Show if on-the-fly data analysis of complex systems is possible by combining:**
  - **a state of the art materials science questions (OPV or Nafion)**
  - **state the art X-ray detectors and instrumentation**
  - **advanced mathematical algorithms and software**
  - **fast data movement and visualization**
  - **run on some of the fastest computer in the world**

A. Hexemer (LBNL/CAMERA), C.E.Tull (LBNL), J. Deslippe (NERSC), R.S. Canon (NERSC), E. Dart (ESnet), I.Foster (ANL), J.A. Sethian (LBNL/CAMERA), G. Shipman (ORNL), J. Wells (ORNL), K. Kleese van Dam (PNNL), T.P. Russell (UMass), E. Gomez (PennState)

Facilities: ALS (BES), NERSC (ASCR), ANL(ASCR), OLCF (ASCR), ESnet (ASCR), CAMERA (ASCR)

How about Real-time?

Experiment:	1 frame per second 600 frames total/sample + 15 min sample change total of 25 min
Time to fit single frame per node (actually 20x same data frame with different initial conditions, since we need statistics) (TITAN and EDISON)	12-20 min

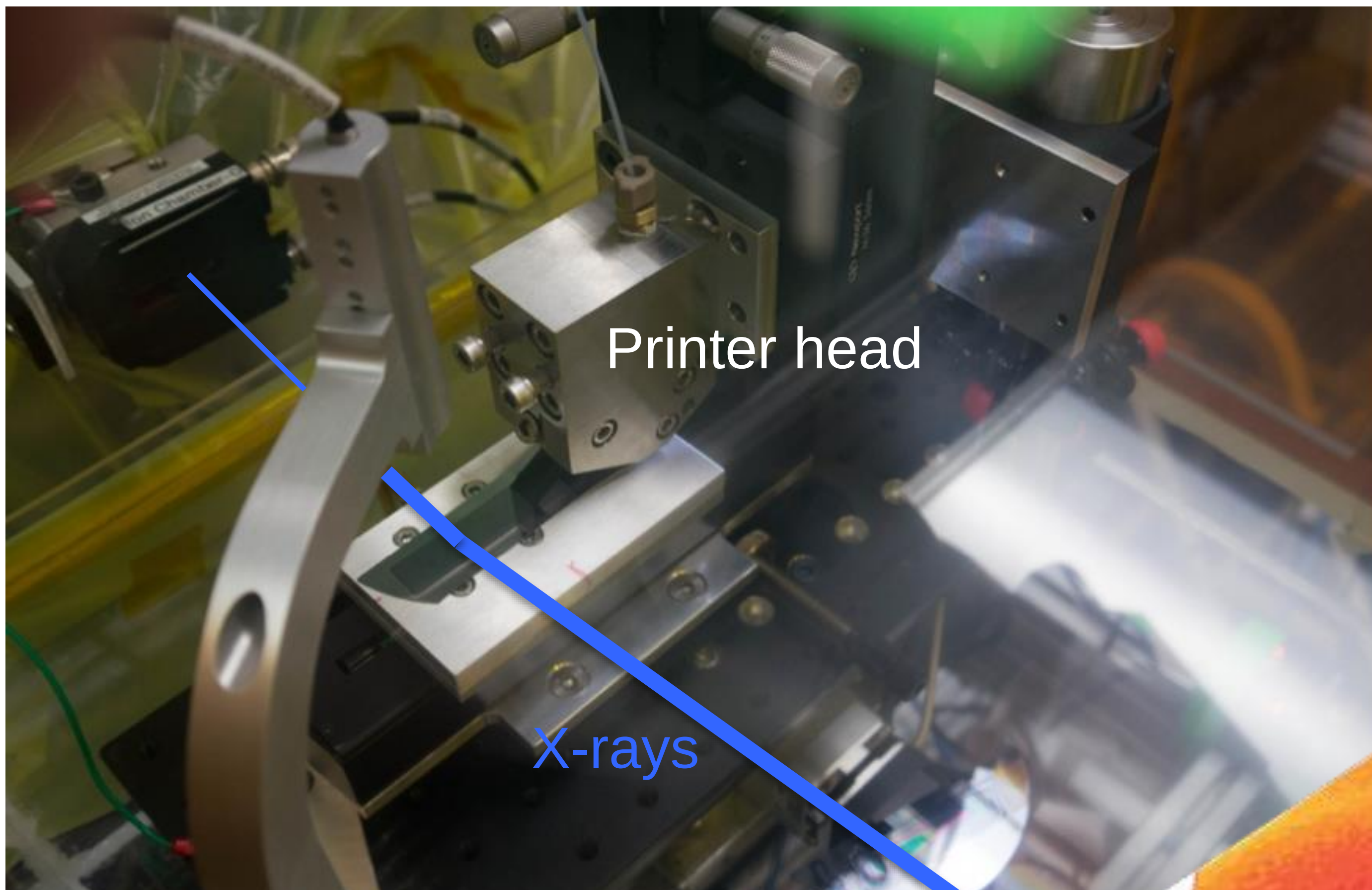
Possible !!!

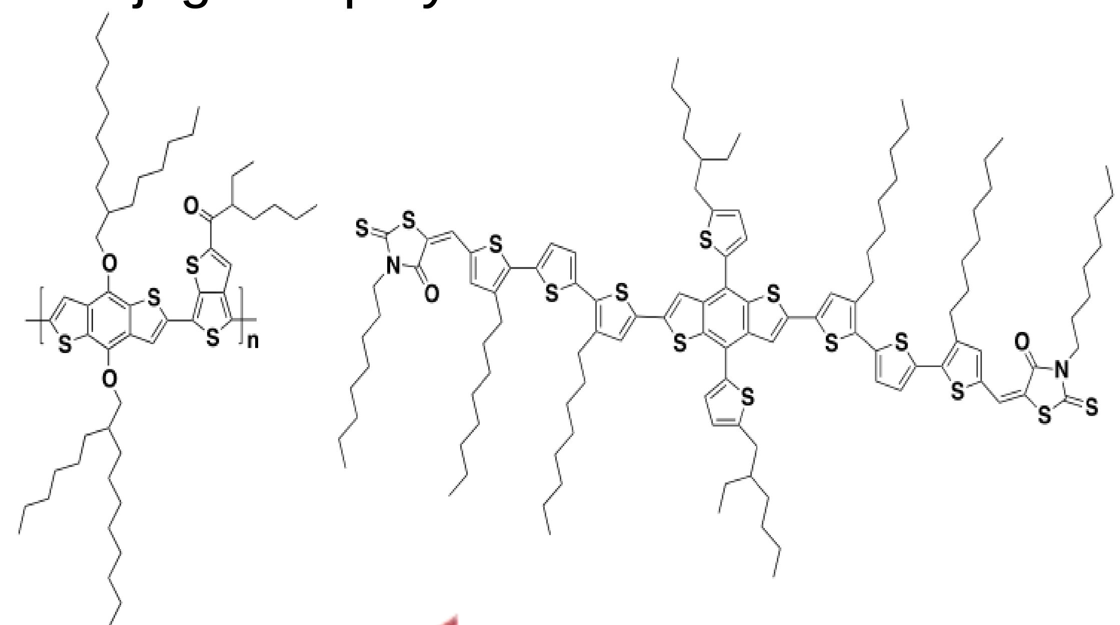
Organic Photovoltaic Processing using Roll-to-Roll

One of the revolutionary appeals of roll-to-roll manufacturing of organic photovoltaics (OPV) is the potential to achieve energy recovery times as low as 10 days. R. Sondergaard et al.: materialstoday Volume 15, Issues 1–2, January–February 2012, Pages 36–49

Conjugated polymer and small molecule

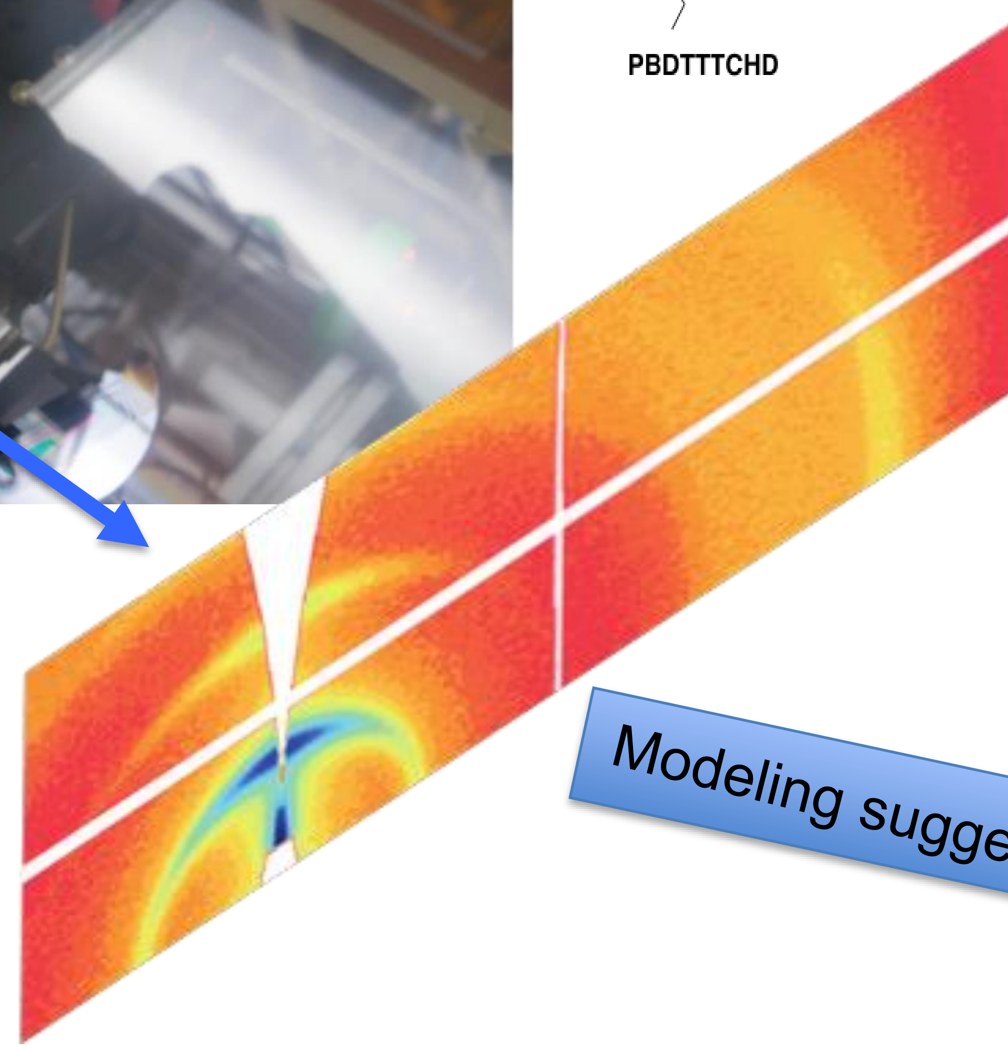
Roll to Roll printer placed inside the beamline





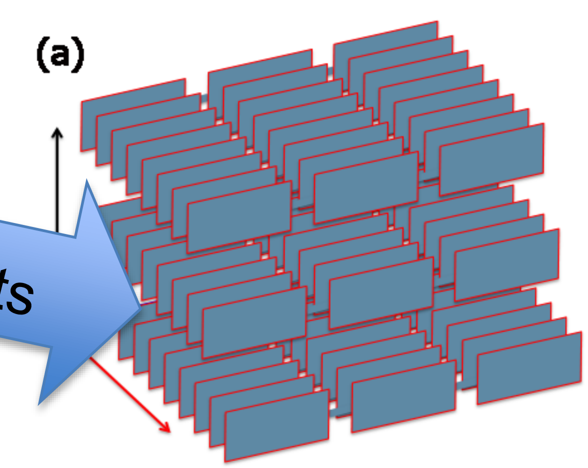
PBDTTTCHD

SMPV1



Edge-on packing

Modeling suggests



GIWAXS data we collected during printing

Real time?

Titan: 1 K20X GPU/node

 # nodes = 500, # agents = 20, # generations = 20:
Total time = 3110.00 sec [avg. generation time = 155.50 sec]

 # nodes = 2000, # agents = 50, # generations = 20:
Total time = 2071.60 sec [avg. generation time = 103.58 sec]

 # nodes = 8000, # agents = 80, # generations = 20:
Total time = 865.60 sec [avg. generation time = 43.28 sec]

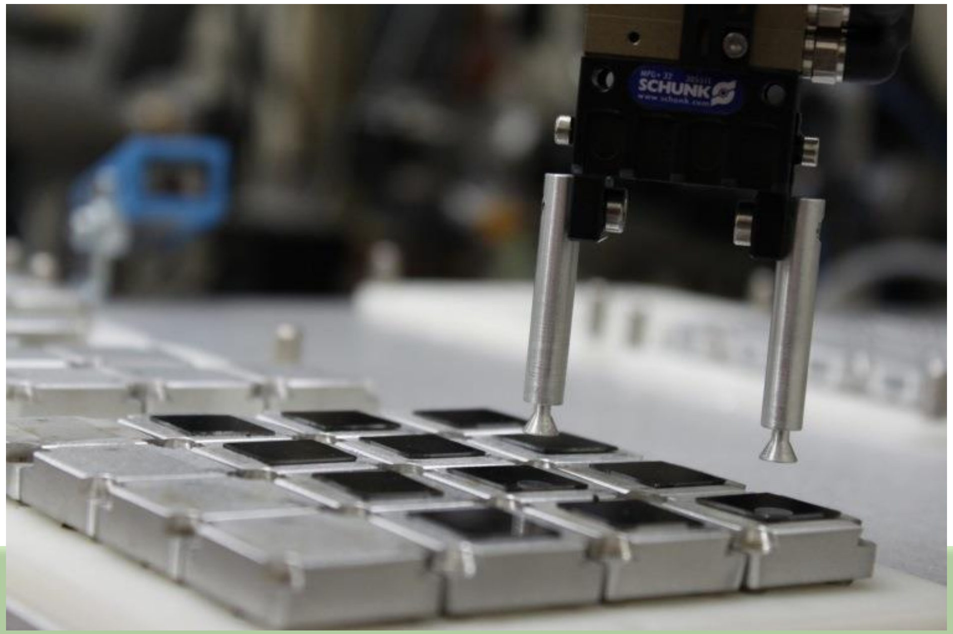
Printing demo experiments created 36,000 frames in 3 days (1/2 year on TITAN)

Sorry for this slide !!!

- Collect all meta data possible into database (none sql)
- Use supercomputer to store, organize, share and analyze datasets (all? just large?)
- use prior information of the materials: How? Easy?
- automate what ever possible: Data reduction, peak finding, fitting, remove background etc. Collect all information immediately.
- Display large datasets: (not as movie, movie has still just one frame at a time) e.g. 3D rendering …
- Analysis tools have to be cross platform and accelerators: Linux is a must for supercomputer, be memory aware: load data on demand not all at once …
- Use modern tools for data: Reduce time/energy/angle series to just essential frames, use machine learning for pattern recognition and see how far we can push it …
- EASY TO USE !!!

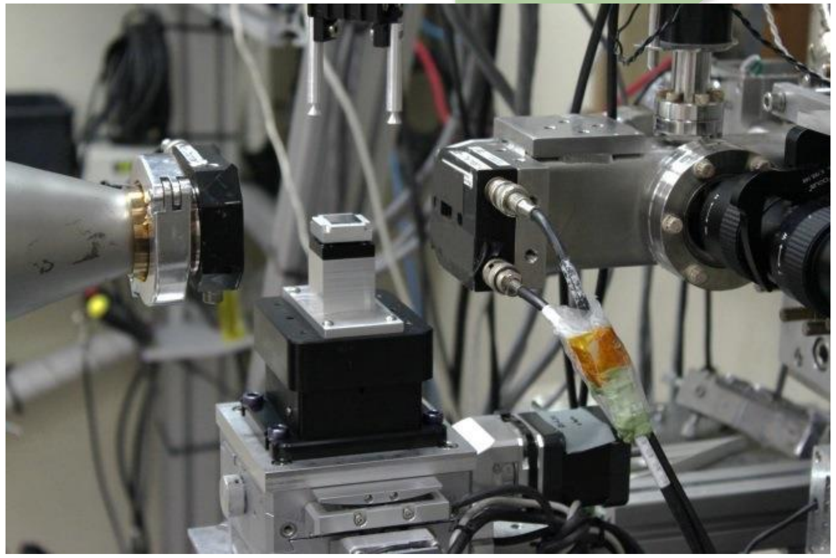
Data Collection: Robot

Epson G6
SCARA robot

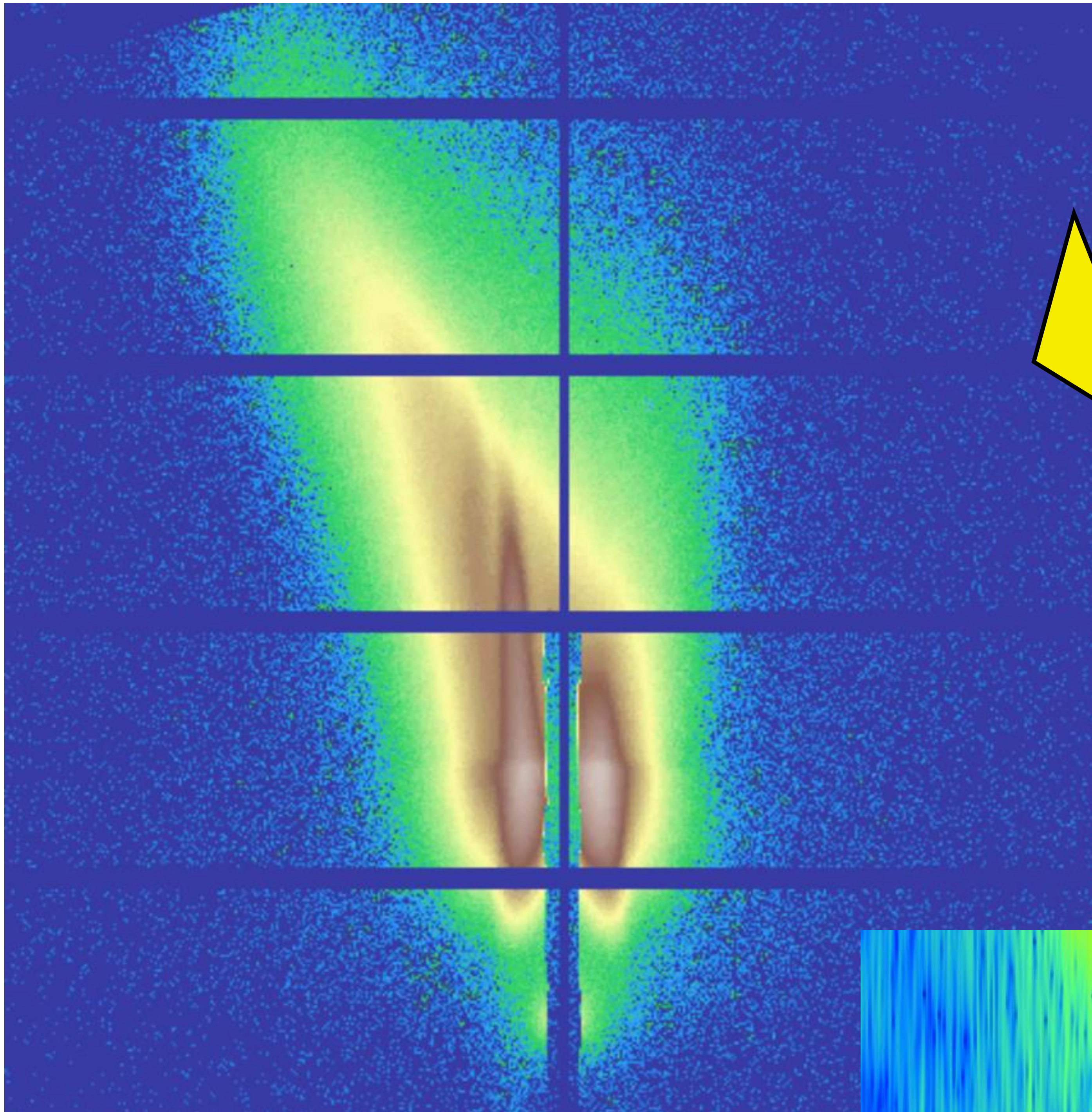


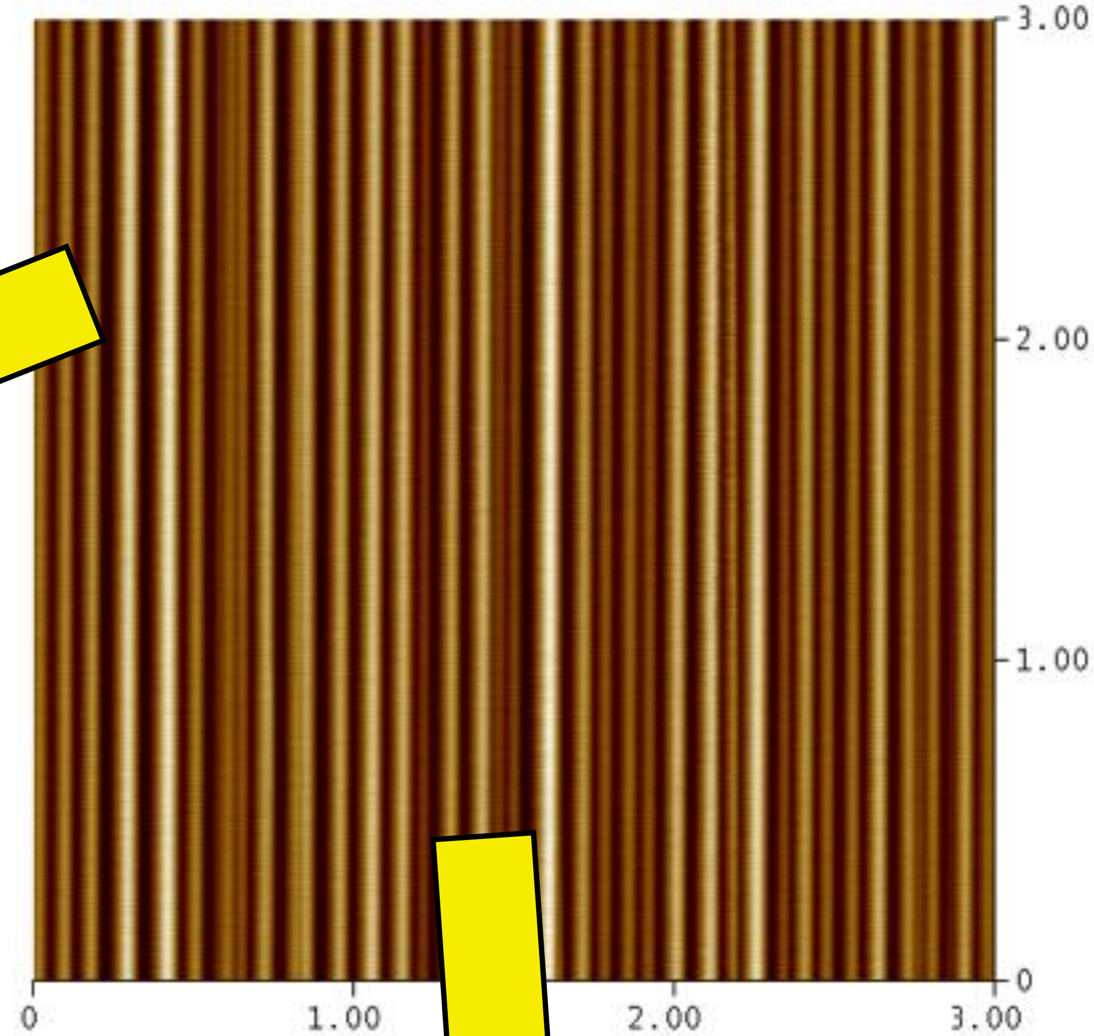
Each puck is a kinematic mount for repeatable, secure transfers

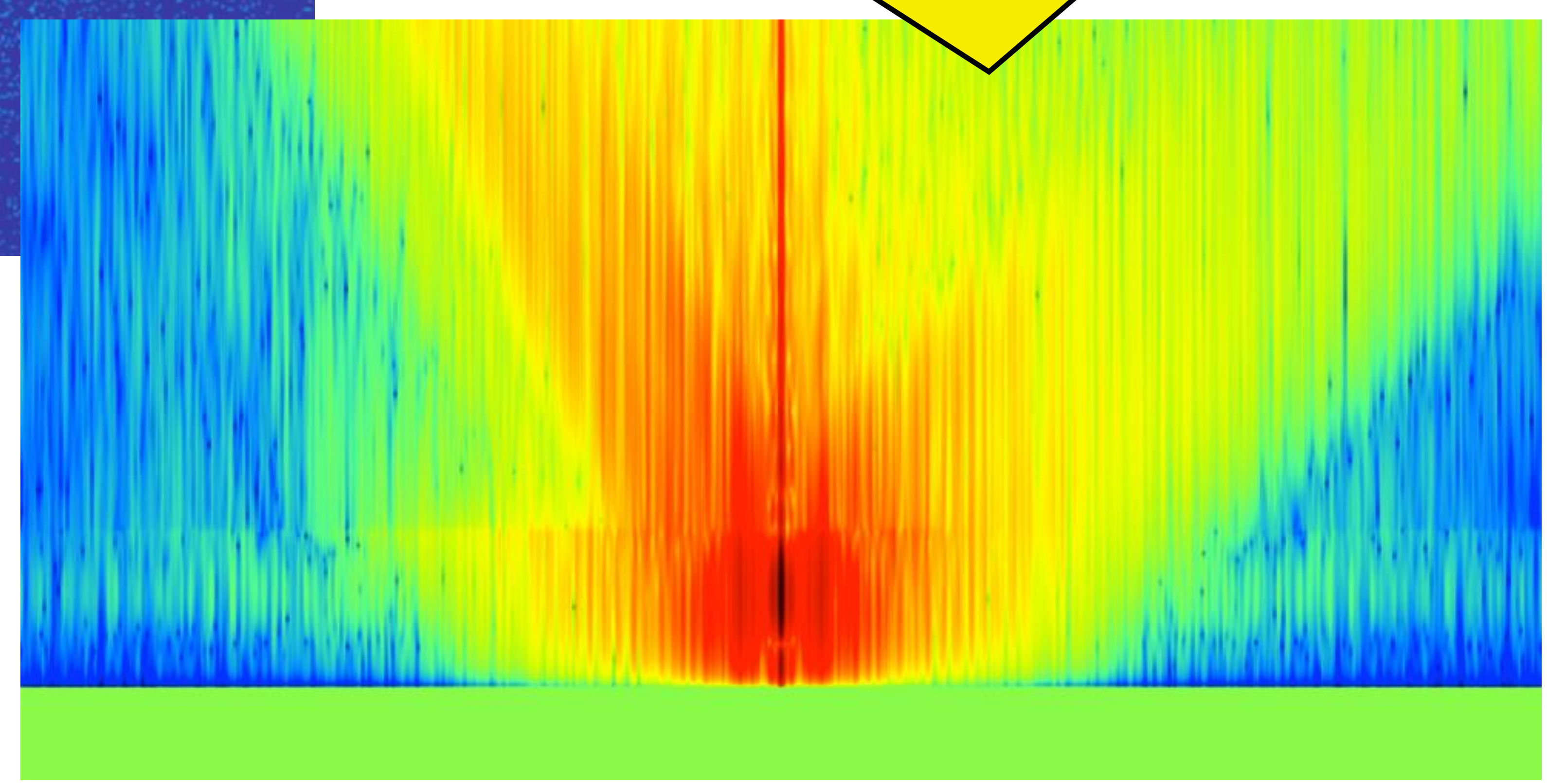
Barcode reader



Measurement stage

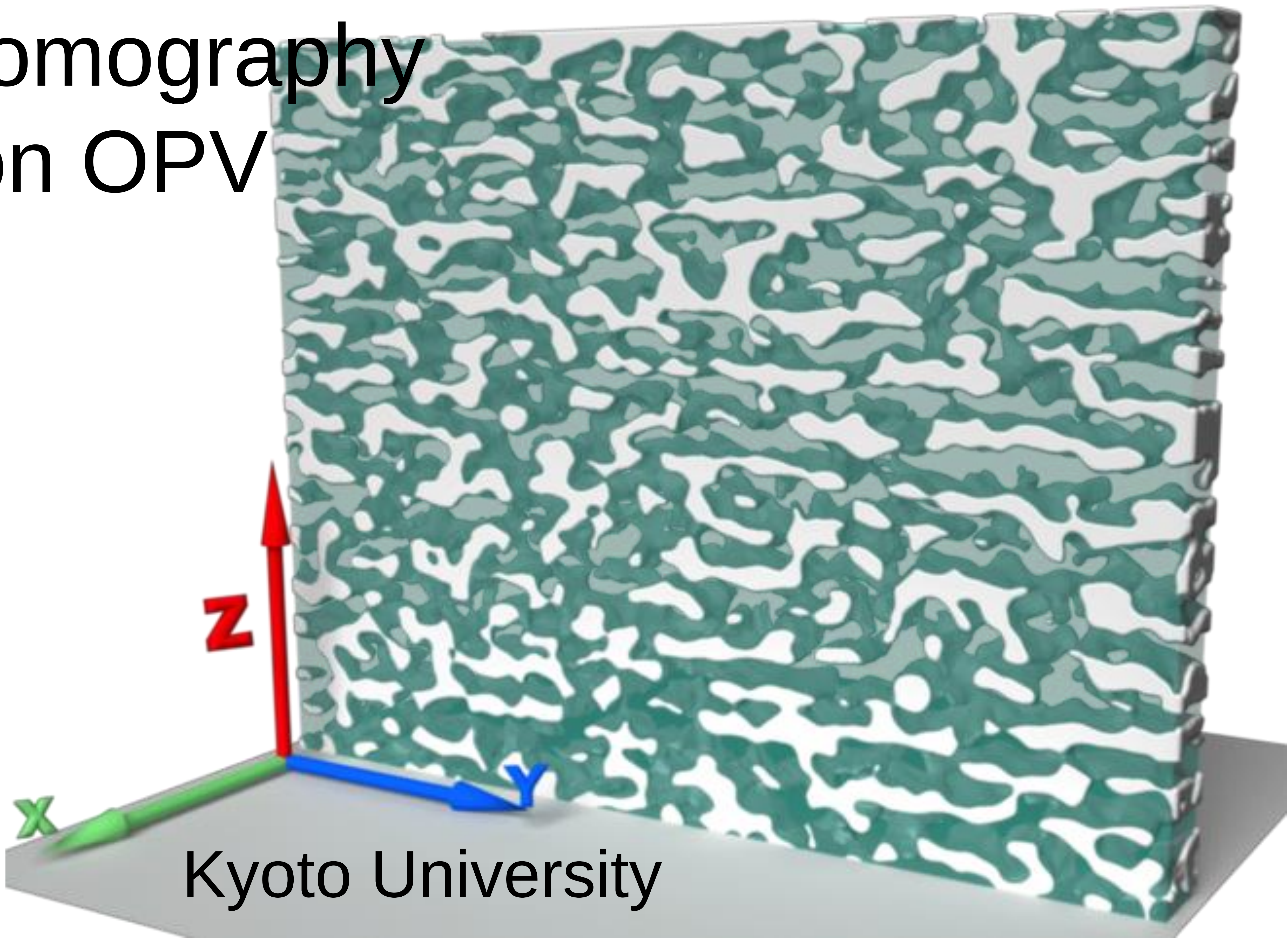






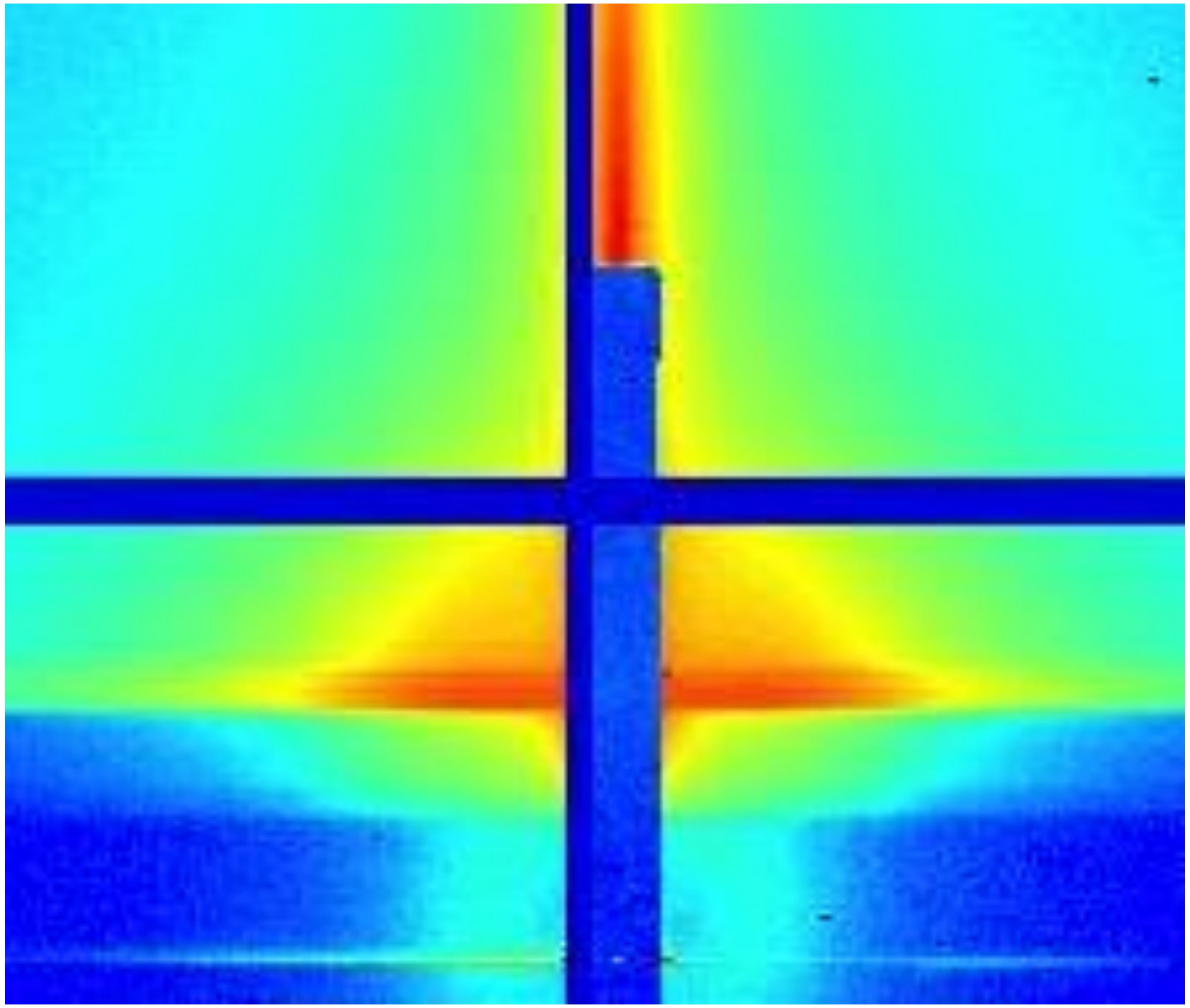
collaboration with
Eric Grohn (Cornell)

Electron energy loss tomography on OPV

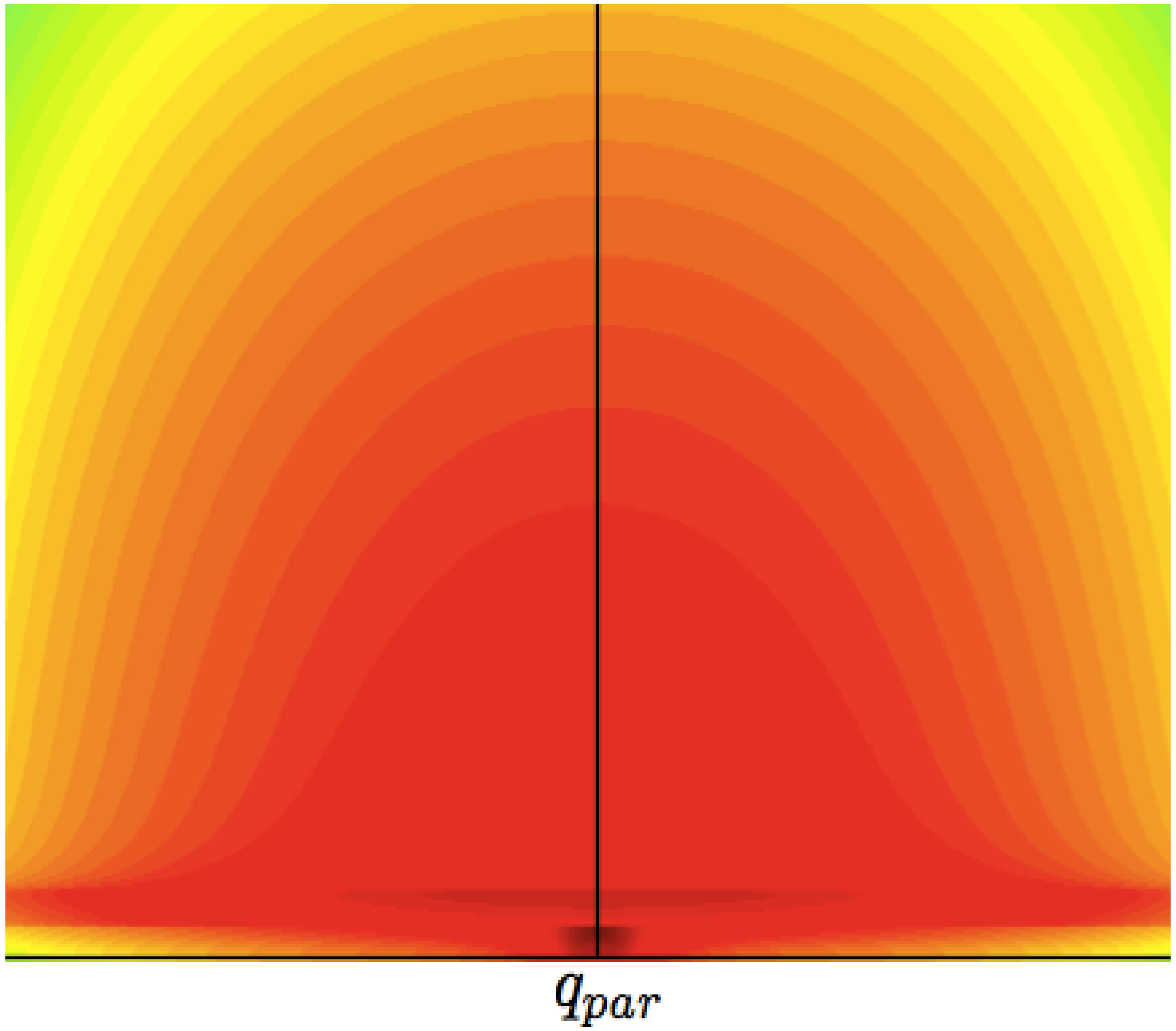


Kyoto University

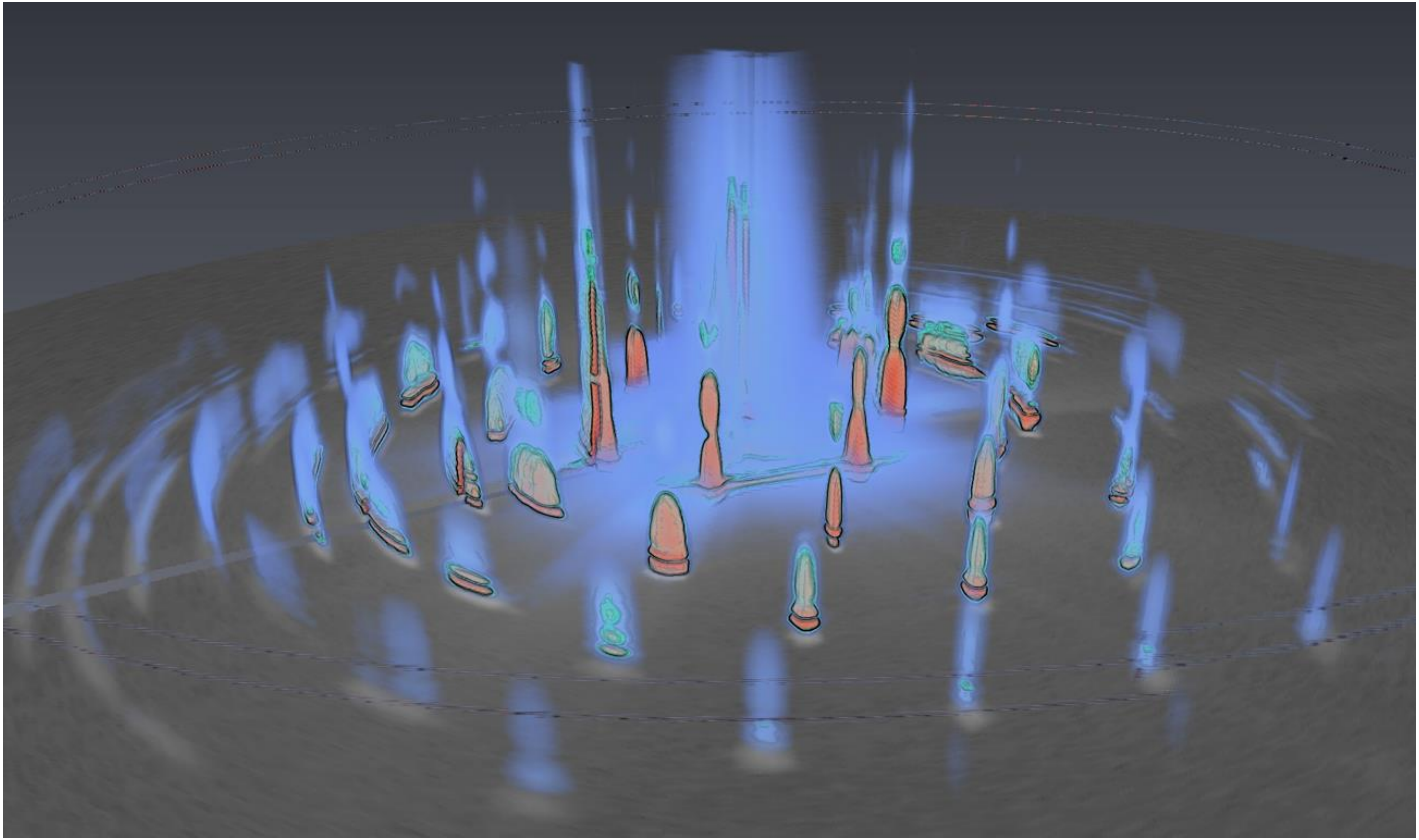
GISAXS from sample set



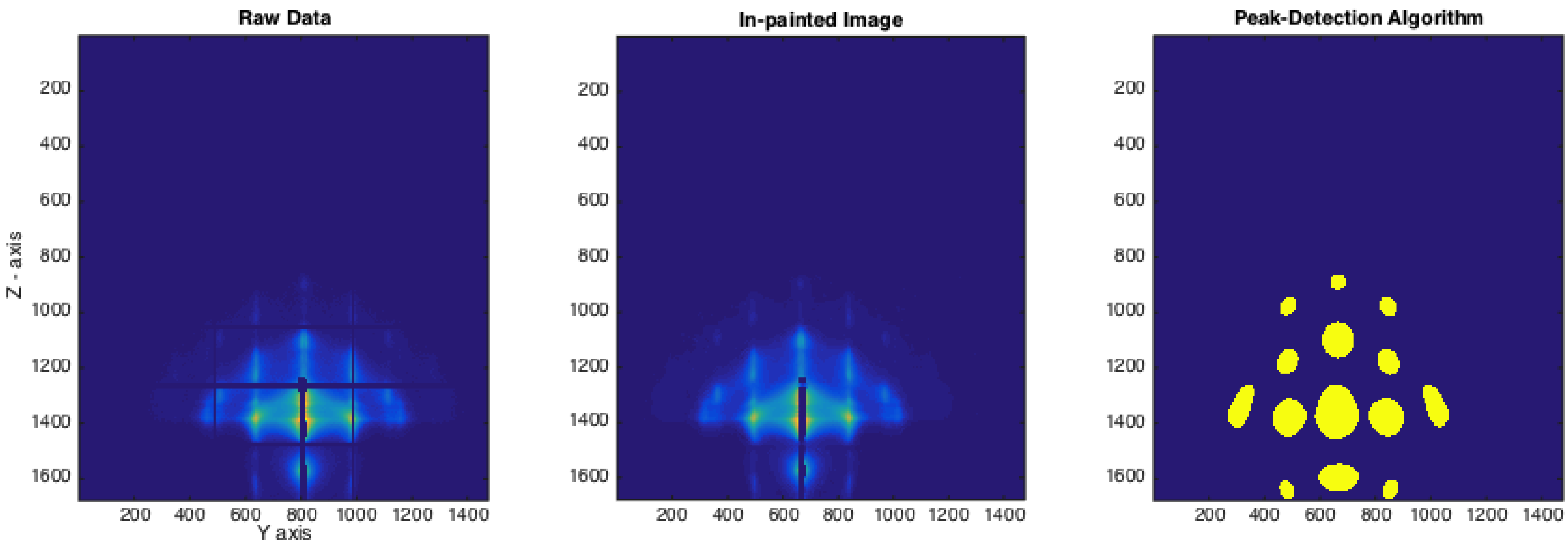
GISAXS simulation from tomography set



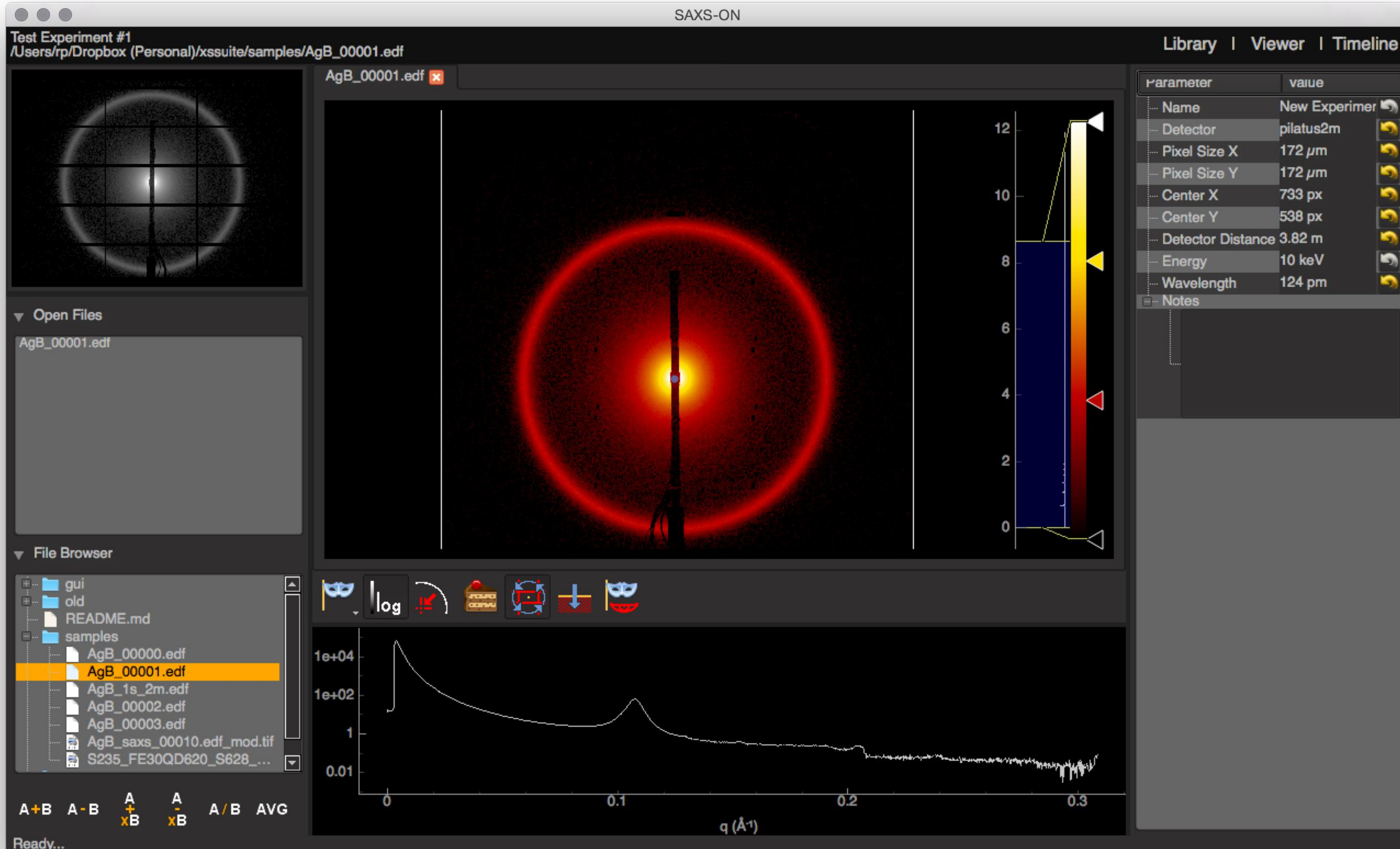
Frame Assembly



can be computationally expensive



Raw Data
In-painted Image
Peak-Detection Algorithm
Z - axis
Y axis
200
400
600
800
1000
1200
1400
1600


SAXS-ON
Test Experiment #1
/Users/rp/Dropbox (Personal)/xssuite/samples/AgB_00001.edf
Library | Viewer | Timeline
AgB_00001.edf
Open Files
AgB_00001.edf
File Browser
gui
old
README.md
samples
AgB_00000.edf
AgB_00001.edf
AgB_1s_2m.edf
AgB_00002.edf
AgB_00003.edf
AgB_saxs_00010.edf_mod.tif
S235_FE30QD620_S628_...
A+B A-B A+xB A-xB A/B AVG
Ready...
Parameter value
Name New Experimer
Detector pilatus2m
Pixel Size X 172 μm
Pixel Size Y 172 μm
Center X 733 px
Center Y 538 px
Detector Distance 3.82 m
Energy 10 keV
Wavelength 124 pm
Notes
log
q (Å-1)