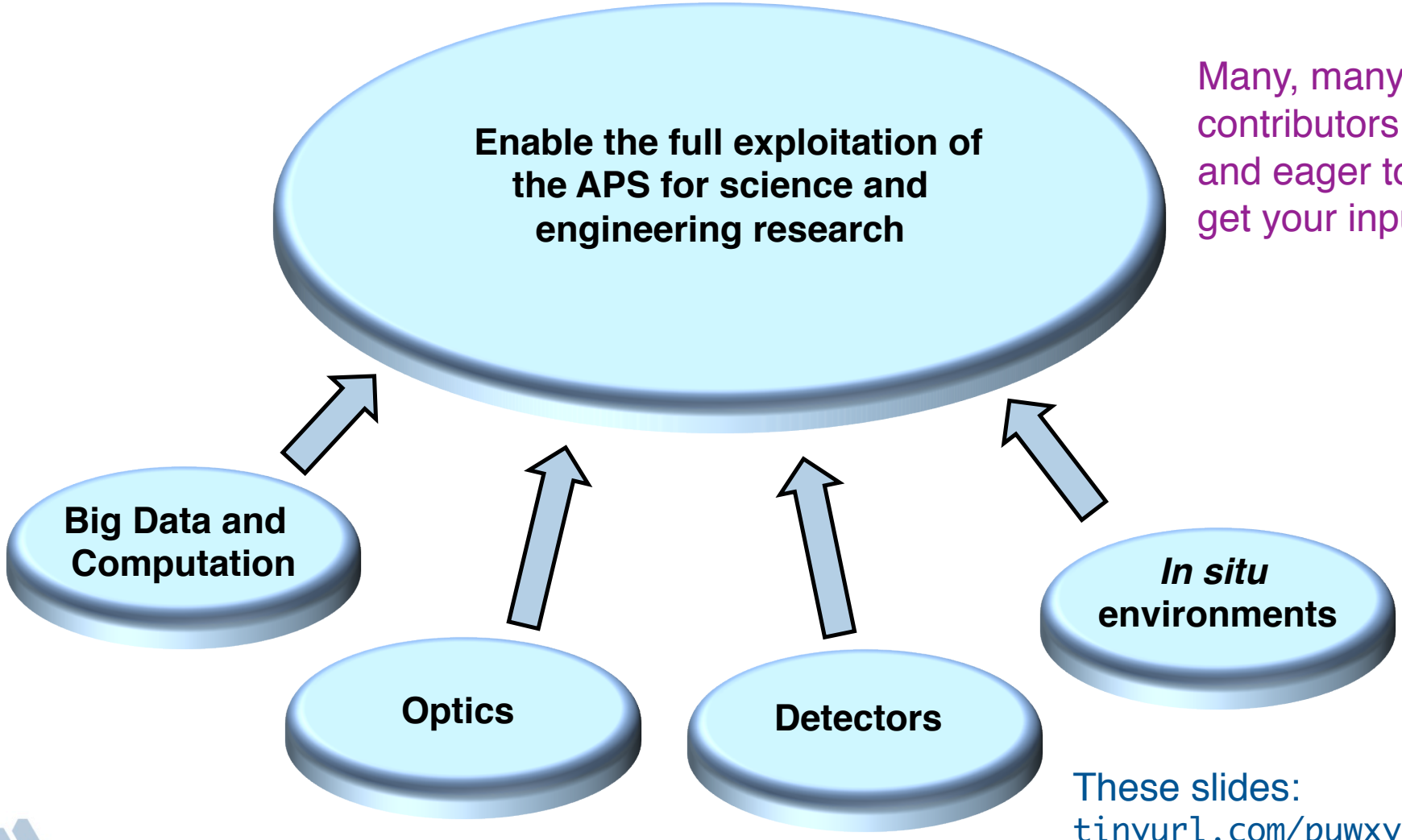
# XSD strategic planning: instrumentation and computing

Where are we today? Where do we want to be in 3 years? Where do we want to be with the MBA lattice upgrade? How to get there?




Many, many contributors - and eager to get your input!

These slides:
`tinyurl.com/puwxy6u`

# Big Data and Computation at the APS: context

- The APS generates 100-300 TeraBytes of data per month today.
  - Among the highest data rates of any US research facility.
  - Dramatic increase with improved detectors, and the MBA lattice upgrade!
- Argonne has great strengths in Computational Science:
  - Machines including Mira (10 petaflop IBM Blue Gene/Q with 768K cores, 768 TB RAM, 35 PB storage) in the Argonne Leadership Computing Facility.
  - Strong researchers in Math and Computer Science at Argonne.
  - Leadership in data transfer with Globus Online; Globus Catalog coming.
  - Center for Heirarchical Materials Design (Northwestern/NIST); Institute of Molecular Engineering (Chicago)
- Our datasets are becoming too large rich to analyze “by examination” – we are entering a new era of employing Big Data methods to discover the whole story that our experiments tell us.
  - “Live” analysis during an experiment can guide us to the next region to examine, or tell us if we have sufficient statistics.
  - “Live” simulation of material properties can help in interpreting results, and point to the next adjustment in environmental or operating conditions while still at the beamline - as well as the next step in material synthesis.

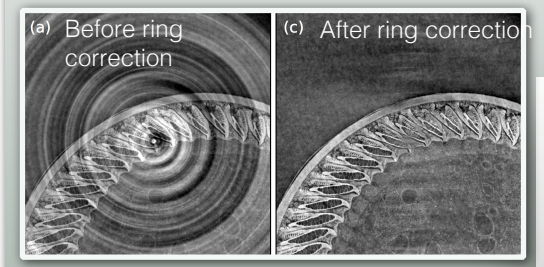
# Big Data today: examples

- Tomography: TomoPy modular framework (Python/C-C++); DataExchange HDF5 files; multi-beamline and modality.
- XPCS: Hadoop map-reduce parallel processing on APS cluster for speedup of 20x (typical) or 50-100x (sparse data).
- X-ray diffraction microscopy: parallel reconstruction of crystalline grain structure. 1-ID and 34-ID.
- X-ray fluorescence microscopy: online quantitation, classification and statistics from images.
- Ptychography: 220x speedup using GPUs, development of improved reconstruction algorithms.
- GSAS/EXPGUI and GSAS-II: crystallographic analysis of single crystal and powder diffraction data.

# TomoPy: Gursoy, De Carlo, Xiao

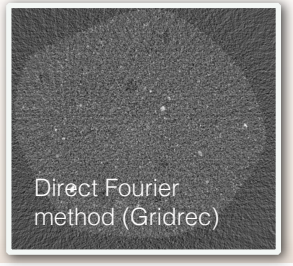
## Data pre-processing

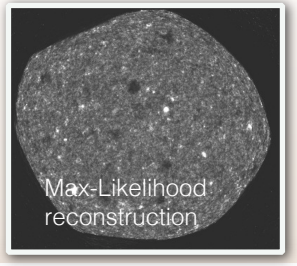
- Correction of rings
- Zinger removal
- Automatic determination of geometric parameters
- Data filtering/padding




## Advanced reconstruction methods

Reconstructions with 46 projections




Iterative model-based reconstruction methods

- Enables fast imaging
- Considerably reduces radiation to samples
- Enables designs of optimal data acquisition

Convex max-likelihood algorithm, ART, implemented with multi-level optimization.

## TomoPy

- Modular open-source development framework
- Python/C-C++
- Platform and data format independent
- Enables off-site data processing
- Ease of collaborative development of scripts

http://aps.anl.gov/tomopy

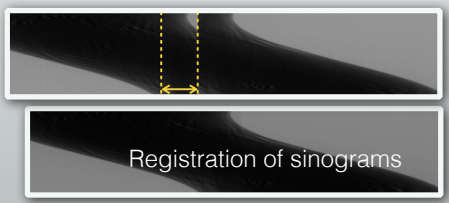
## Data registration and fusion

Integration of micro-CT, nano-CT and X-ray Fluorescence-CT... plus more?

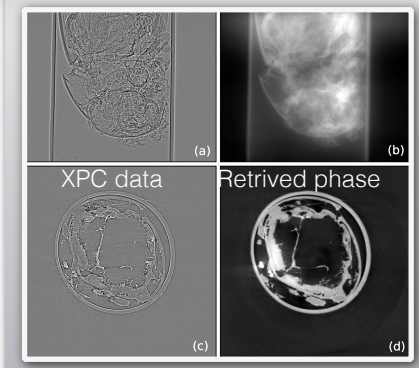
- Geometry registration
- Region-of-interest tomography
- Integrated image reconstruction
- Constrained optimization and data fusion

Field-of-view-correction:

- Allows imaging of samples larger in size than the field of view of the detector




## X-ray phase retrieval




## Data integration

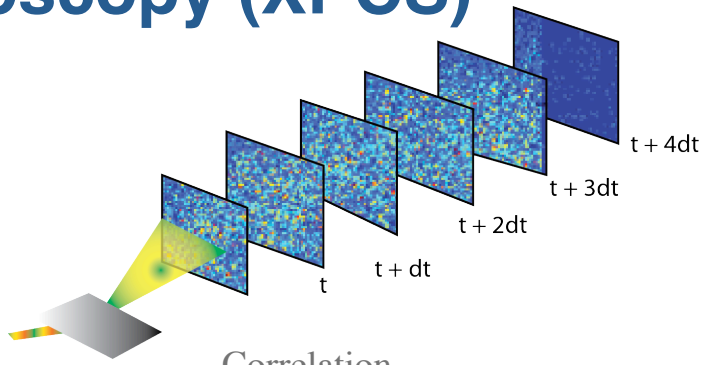
The *Data Exchange* module can import data from

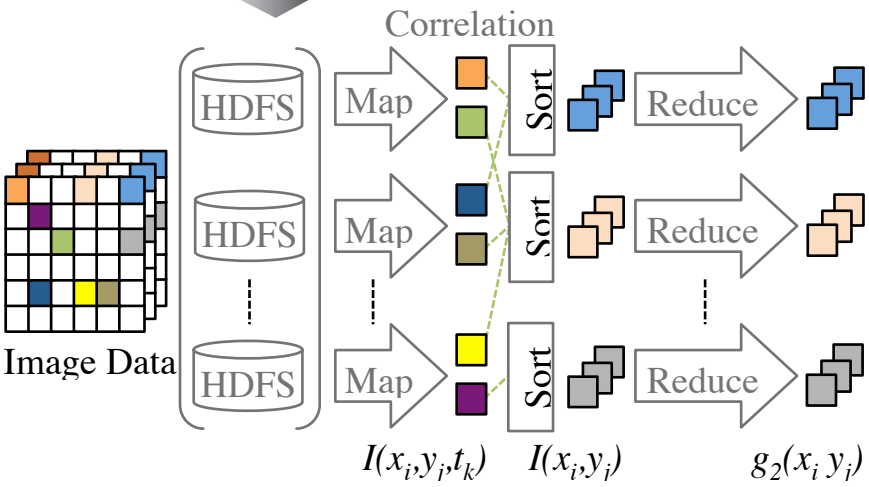
- APS, (*US*) 13-BM, 1-ID, 26-ID, 2-BM
- Anka, (*DE*)
- Australian Synchrotron, (*AU*)
- Diamond, (*UK*)
- ESRF, (*EU*), 19-ID
- Elettra, (*IT*)
- NSLS, (*US*)
- Petra III, (*DE*)
- SLS, (*CH*)

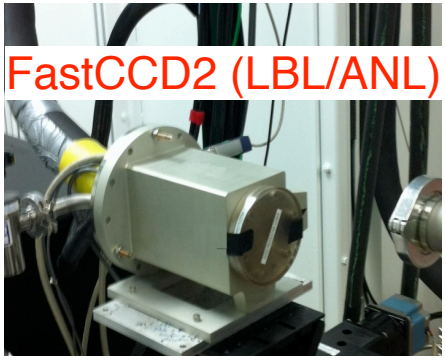
http://www.aps.anl.gov/DataExchange/

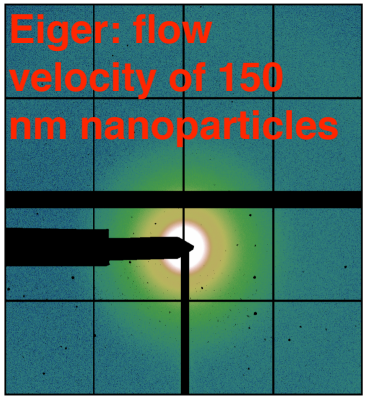
# X-ray Photon Correlation Spectroscopy (XPCS)

- Commercial CCD: 1Kx1K @ 60 frames/sec.
- FastCCD2: 0.1x1K @ 1000 frames/sec.
- Eiger (test): 1Kx1K @ 800 frames/sec, with potential for 3000 frames/sec
- Hadoop map-reduce on 96 cores yields near-real-time analysis (20x speedup typical, 50-100x on sparse data).
- When do I have good enough statistics to stop the experiment?



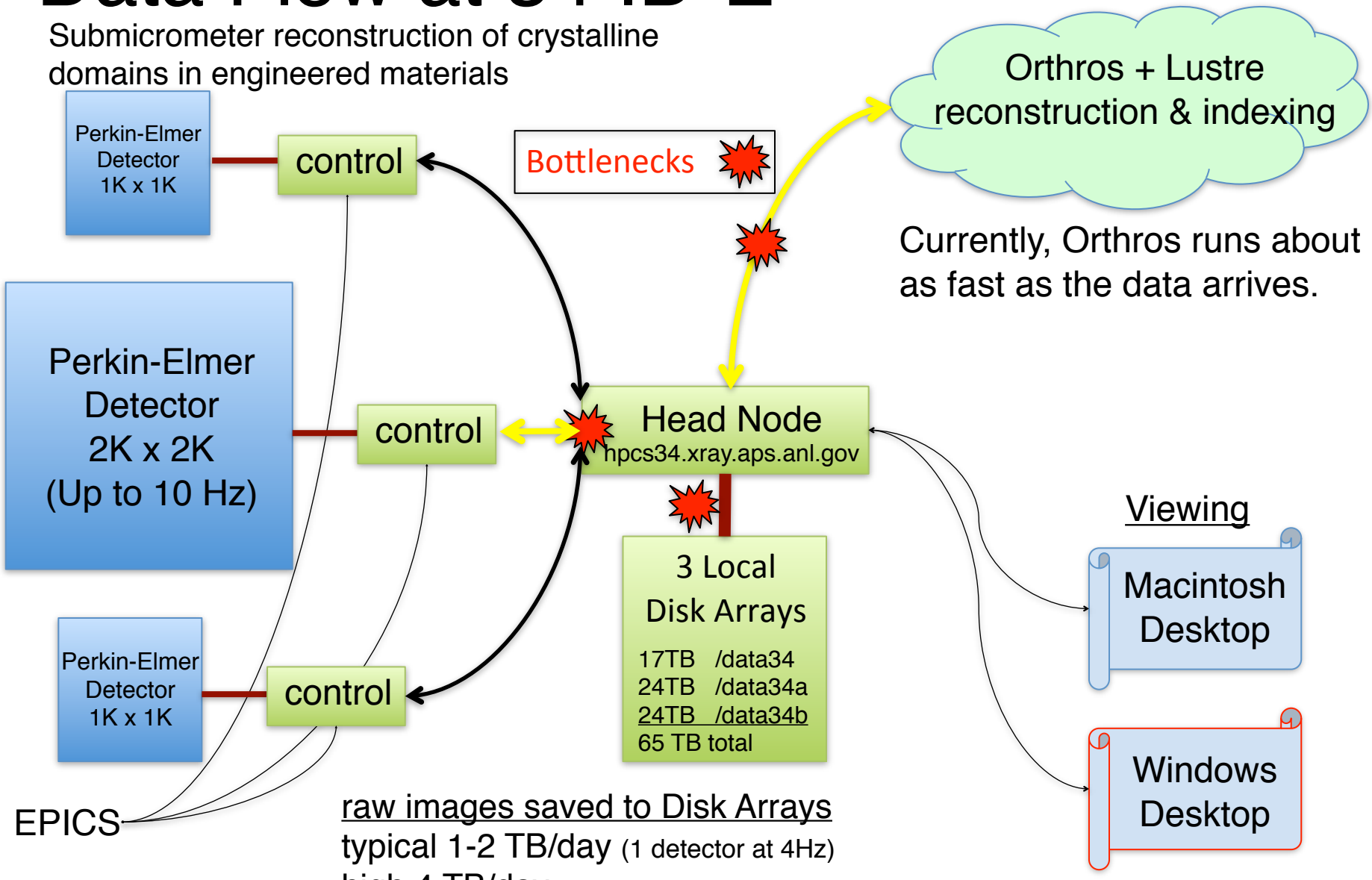



# Data Flow at 34 ID-E

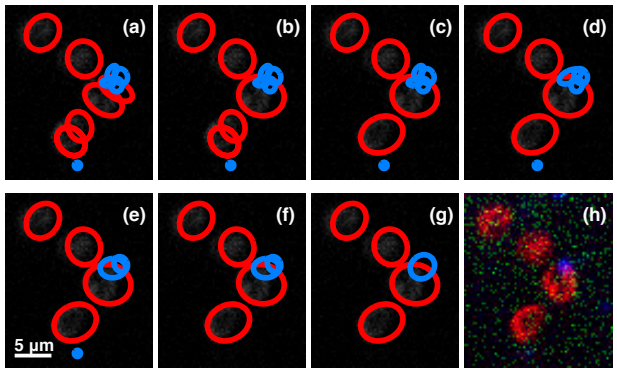
Submicrometer reconstruction of crystalline domains in engineered materials




raw images saved to Disk Arrays
typical 1-2 TB/day (1 detector at 4Hz)
high 4 TB/day
Goal 10 TB/day (3 detectors at 10 Hz)

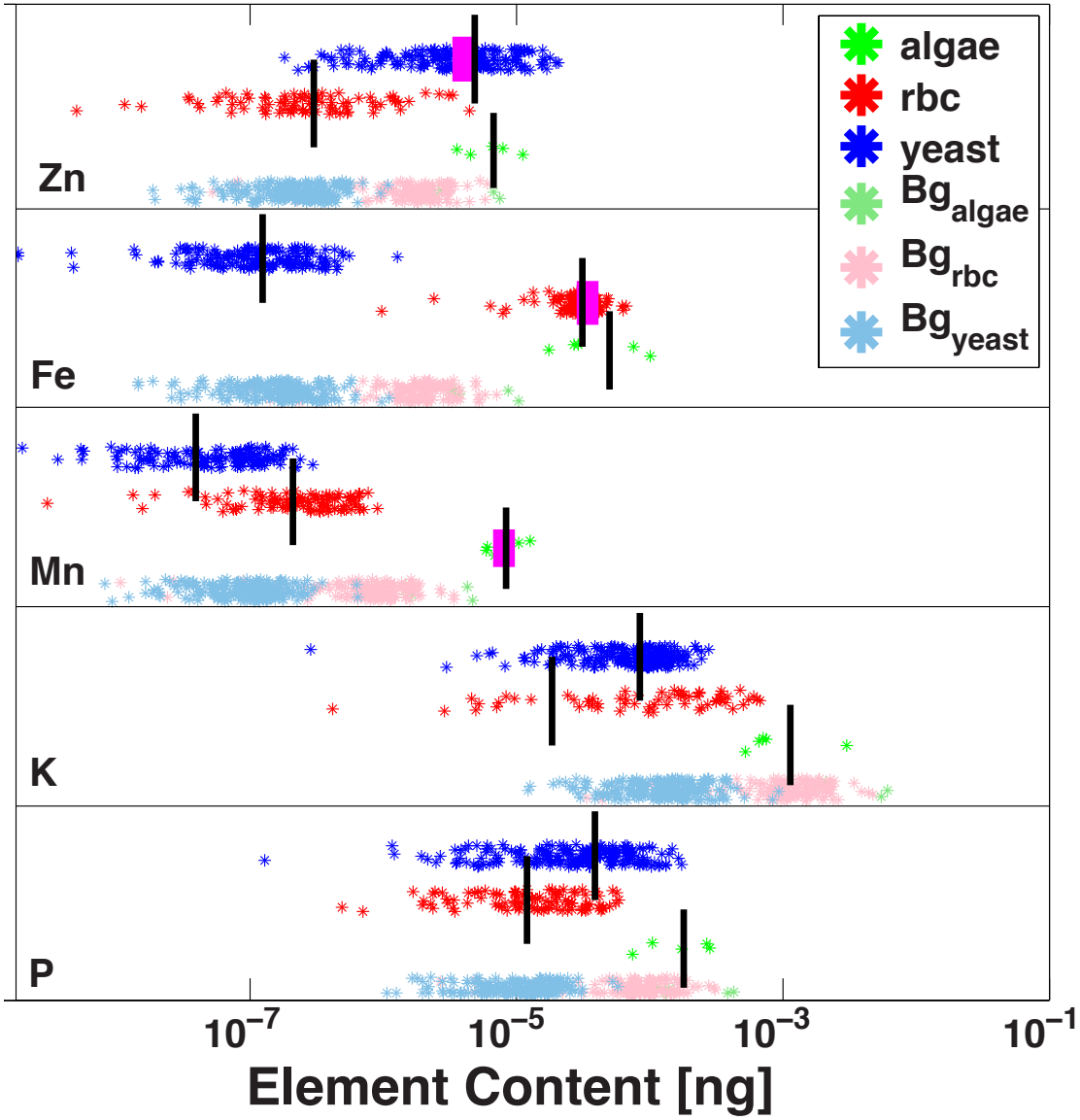
# X-ray Fluorescence Microscopy: images to information

- Fly scans enable rapid acquisition of large pixel count images
- Automatic cell identification, allowing for overlaps.
- Wang, Ward, Leyffer, Wild, Jacobsen, and Vogt, *J. Synch. Rad.* (in press) doi:10.1107/S1600577514001416

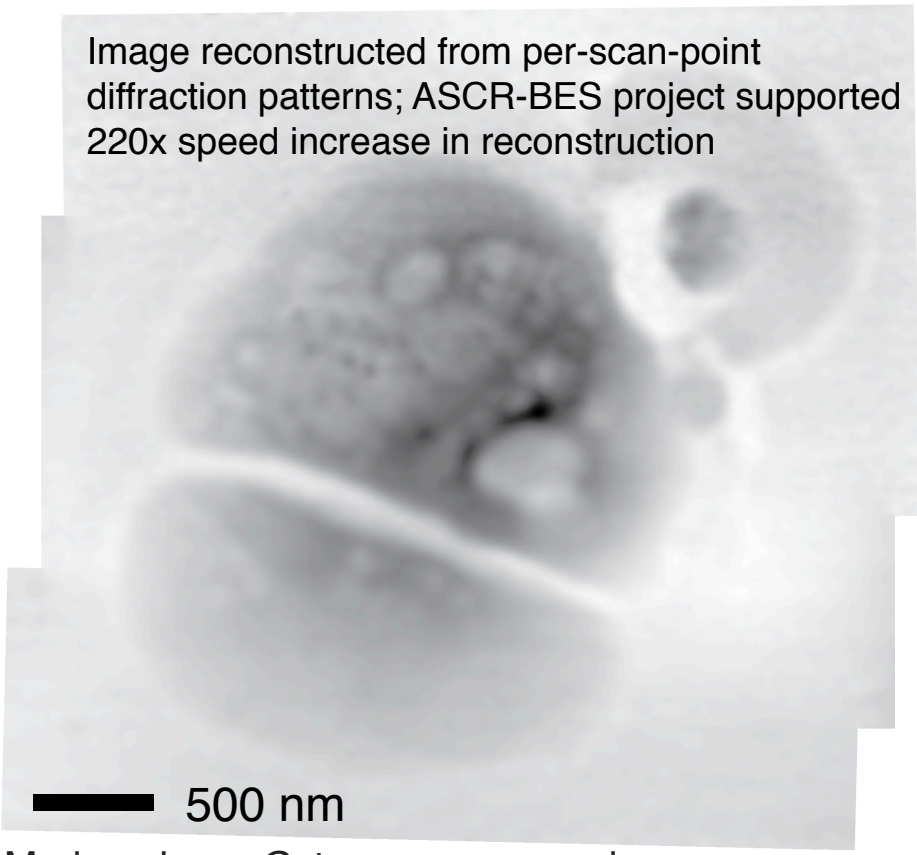


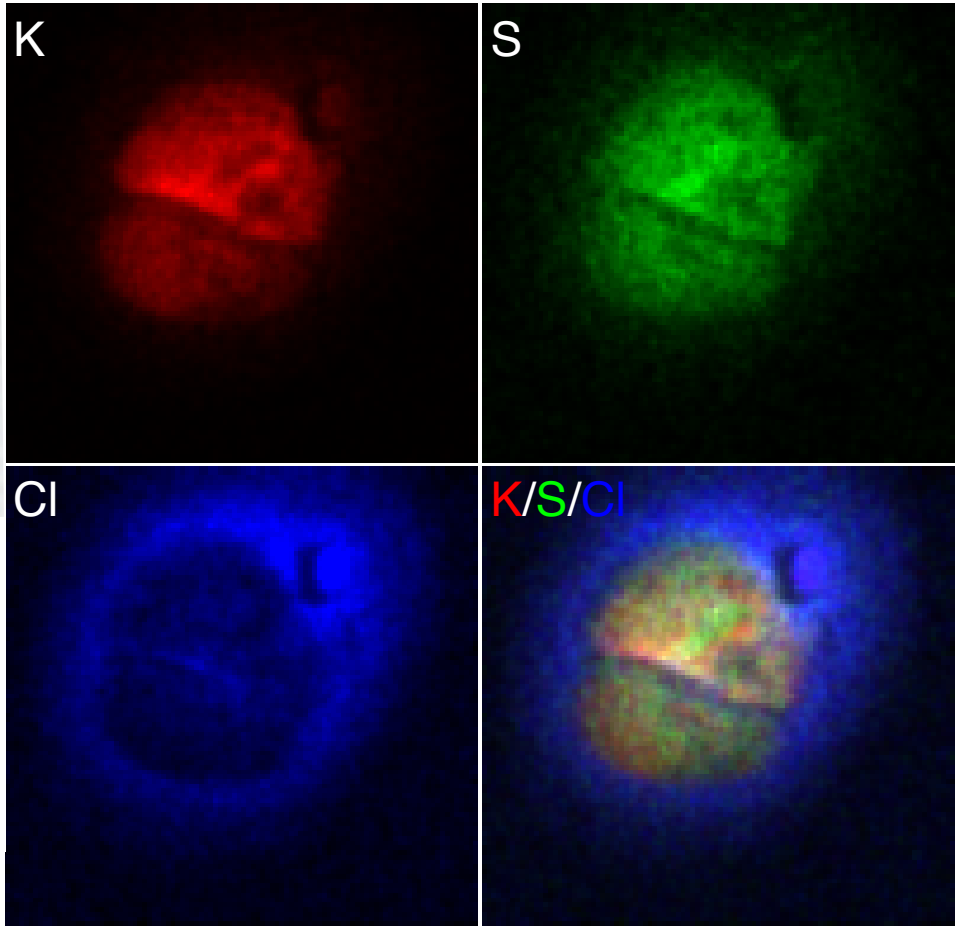

Demonstration on mixed cell sample

rbc=red blood cell



# Ptychography and fluorescence: structure, and chemistry



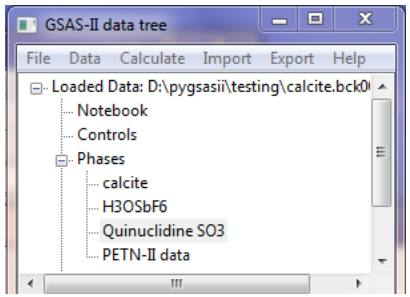

1 µm

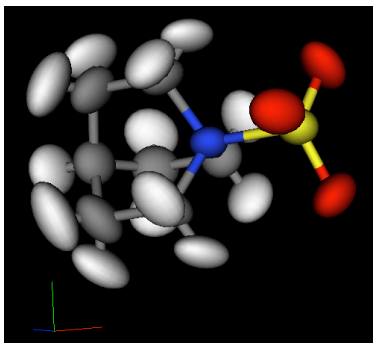
Marine algae: *Ostreococcus* sp., class *Prasinophycae*, common name chlorophyta. Imaged frozen hydrated, at 5 keV photon energy, with 12 nm reconstruction pixel size

First combined cryo high spatial resolution ptychographic image simultaneous with elemental maps from x-ray fluorescence. Junjing Deng, David Vine, Youssef Nashed, Tom Peterka, Rob Ross, Si Chen, Qiaoling Jin, Chris Jacobsen. Argonne Lab/ Northwestern University. BioNanoprobe, LS-CAT beamline.

# GSAS/EXPGUI and GSAS-2: crystallographic analysis

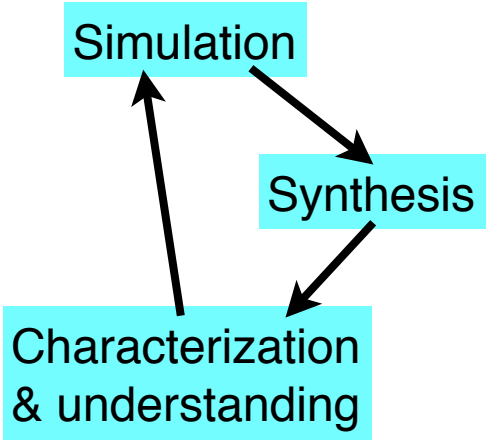
- Single crystal and powder data from x-rays and neutrons.
- GSAS (Larson and Von Dreele) has ~6000 citations; ported to modern computer architectures.
- EXPGUI (Toby 2001) provides graphical user interface and add-on tools; ~2400 citations.
- GSAS-2 (Toby and Von Dreele, 2013) modernizes code base, adds area detector data reduction, indexing, structure solution, small angle and PDF computations.
- Goal: novice-friendly, but expert-efficient; from perovskites to proteins. Reads data from relevant APS beamlines, but also used to analyze data from Mars Curiosity rover.



# Big Data at the APS: roadmap

- Where in 3 years?
  - Automated data management at some beamlines
    - Automatic transfer from beamline computer to central store
    - Automatic first-pass analysis (technique specific)
    - Organization and access via users on ESAF
    - Globus Online distribution, and Globus Catalog search.
    - Pilot project via Tao of Fusion LDRD.
  - Near-real-time discovery from data at some beamlines - to find and follow up on surprises during beamtime!
  - Near-real-time comparison with simulations at some beamlines
    - Example: DFT ⇄structure x-ray scattering (Bachir Aoun, Chris Knight)
- Where with MBA Upgrade?
  - Combined detector-computer-storage pathway for high throughput area detectors, and automated management.
  - Single data access method for all APS beamlines.
  - Real-time data discovery, and comparison with simulations.
  - On-demand launching of virtualized servers for specialized analysis programs? Analysis using APS-curated tools available at users home institutions?

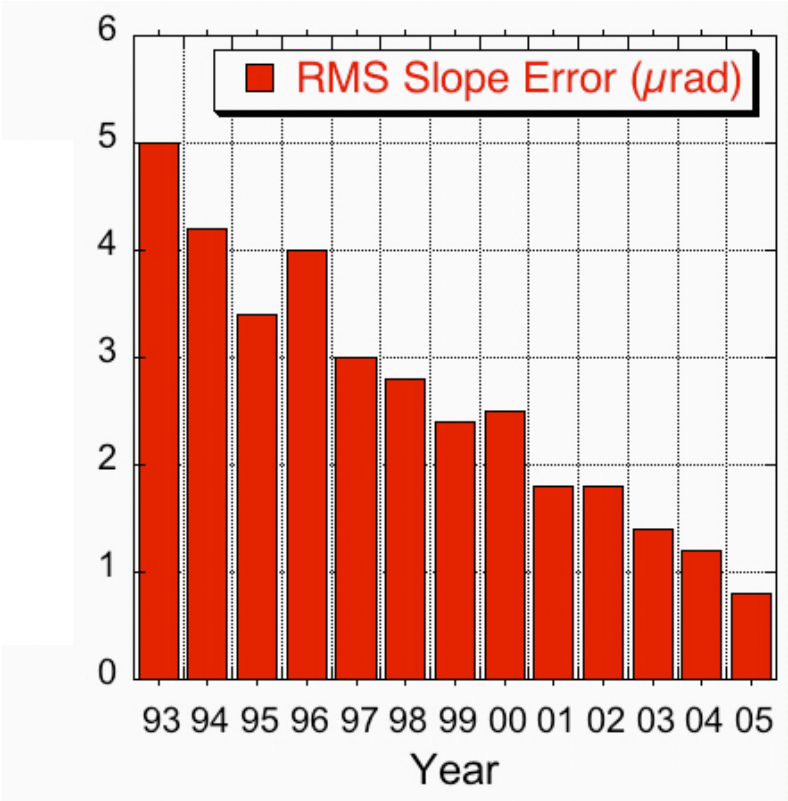


# Big Data: realizing the vision

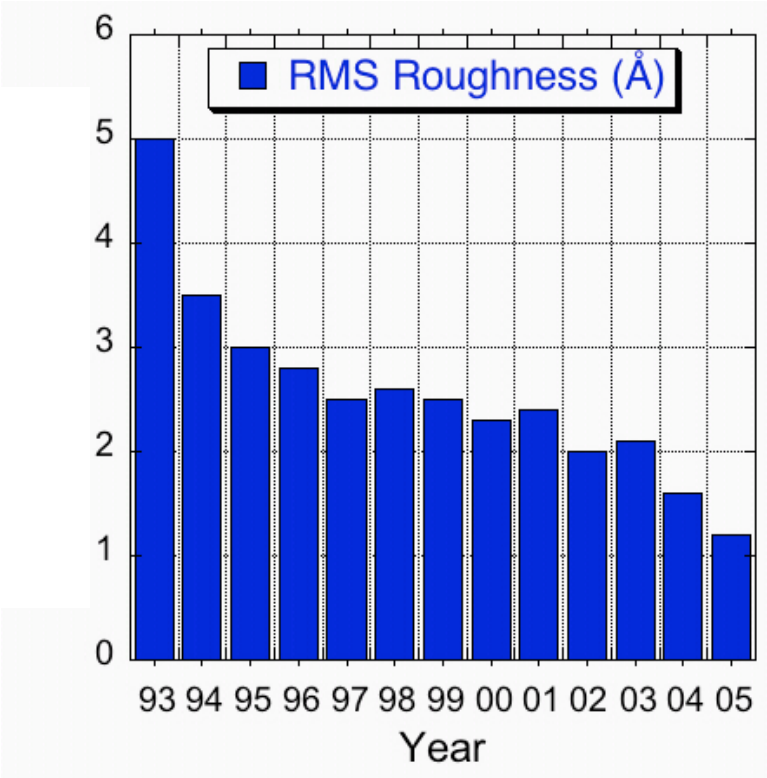
- Argonne has strengths in high-end computing hardware - but we want on-demand, easily accessible, data-already-there...
  - Present solution: APS high performance cluster (HPC; not without challenges). How much should the APS invest in HPC?
  - We need to manage the data in order to analyze the data.
  - Is cloud computing (on-demand virtualized servers) all hype, or will it be a revolution like the transition from mainframe to desktop computing?
- Argonne has strengths in people: computer science and applied math.
  - AES Software Services Group is 4-5x oversubscribed.
  - Symbiotic mutual exploitation for funding (LDRD, DOE/ASCR, DOE/BES, NSF, NIH...). Ptychography already mixes ASCR, BES, NIH.
- X-ray scientists should be leading team approaches, to make sure that solutions are on-target.
  - Integrated approach involving data acquisition, management, reduction, analysis, simulation... e.g., Big Data, Imaging Initiative LDRD call.
  - Should BCDA and SSG be part of XSD?
  - High-level coordination of activities of Buildings 240 and 401?

# Optics: mirror history

Need <0.05 µrad for MBA lattice. Today: manufacturer specs at 0.1-0.2 µrad rms, except JTEC at 0.03 µrad rms.




Need <1 Å rms for MBA lattice



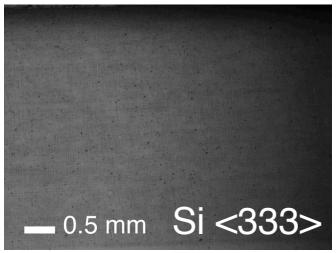

- Compiled from APS and ESRF data (L. Assoufid; ESRF data supplied by A. Vivo)
- Mirror materials: Si, ULE Glass, Fused Silica, Zerodur (1 m long or larger)
- Mirrors acquired from various vendors

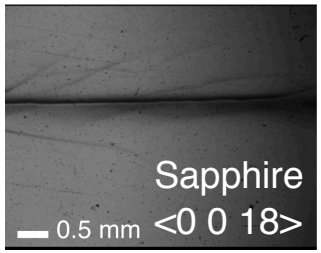
# Optics: context

- APS has had in-house capabilities from the beginning
  - Production of crystal optics (300 delivered last year!) for APS and DoE-wide use. R&D towards <1Å rms polishing for strain-free crystals, plus modeling and analysis.
  - Thin film deposition, including mirrors and multilayers.
  - Characterization including mirror metrology and laboratory topography.
- Significant increase in capabilities!
  - New team in optics and beamline simulations.
  - New, best-in-class long trace profilometer with 0.05 µrad resolution.
  - New Optics and Detector Test beamline (50% of 1-BM) with at-wavelength interferometry and crystal topography.
  - Lab topography resolution improved from 1.0 to 0.1 µrad.
  - New deposition systems for profiled coating.
  - Delivery of optics *systems* (8-BM K-B microfocusing system, including focus characterization).
  - New efforts in ion beam figuring and profiling, and crystal etching and polishing.

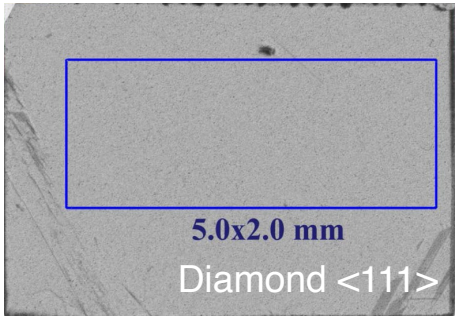
# Optics: emerging initiatives

- Topography, and at-wavelength grating interferometry: crystals, windows, mirrors.

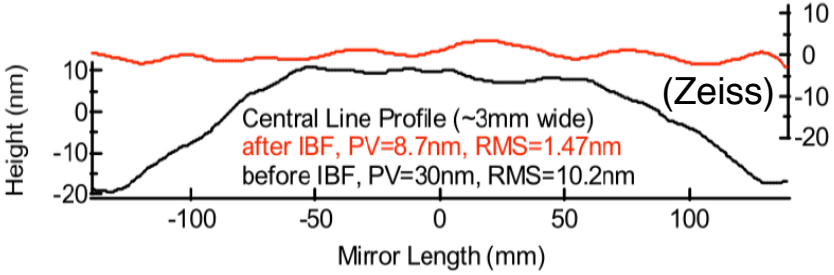


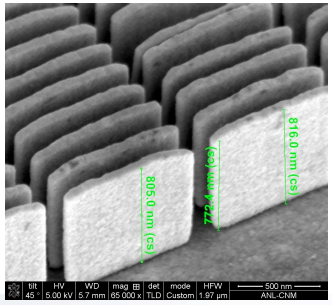

- Low-defect single crystal diamond (with Technological Institute for Superhard and Novel Carbon Materials, Moscow)

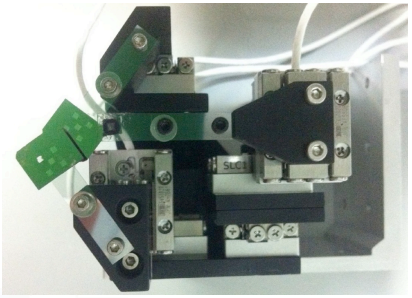



- Metrology⇔profiled deposition to improve existing mirrors



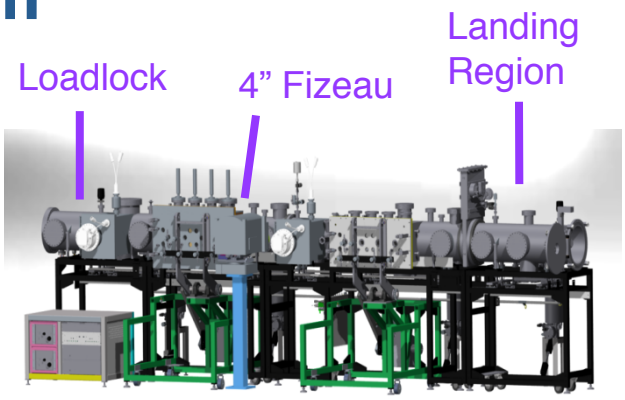

- Nanofocusing with high efficiency: stacked zone plates, and multilayer Laue lenses

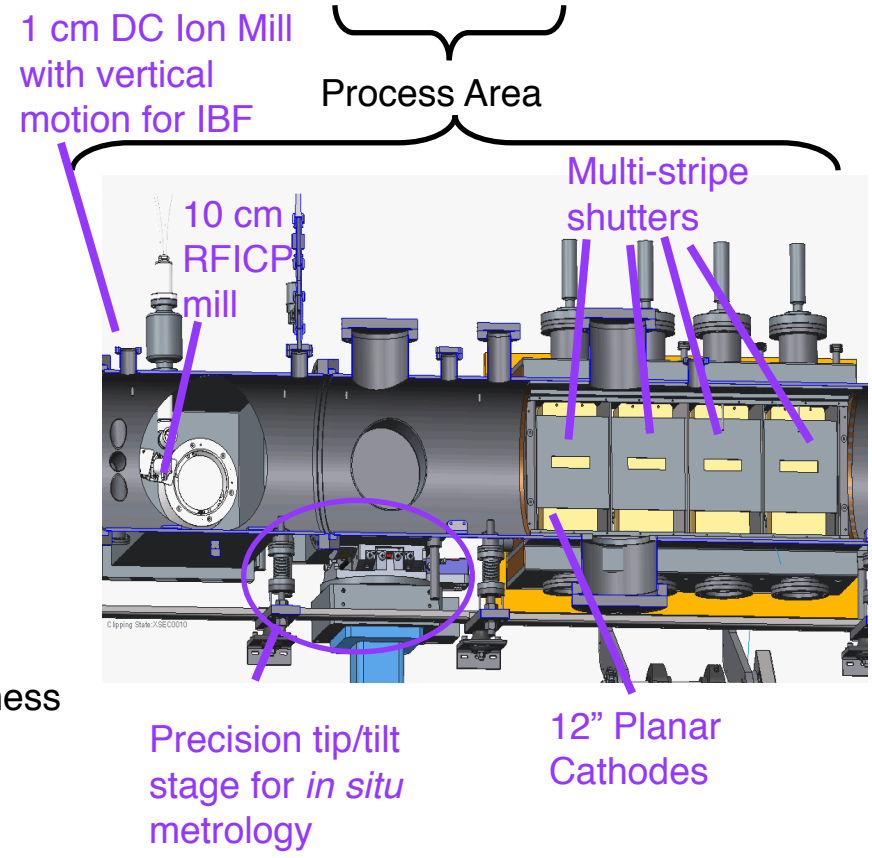




# Modular Multilayer/Mirror System

- New "modular" system design accommodates ion milling, in-situ metrology, and future cathodes
- Metrology+figuring of 15 older APS mirrors justifies the cost of the machine
- The new APS machine can have a broad impact.
  - The BNL machine is for MLL only
  - 12" planar vs. 3" dia. Cathodes (no growth rate drift)
  - Precision multiple reactive gas mixing
  - *In situ* metrology capable
  - Dynamic aperture capable (3-D film gradients)
- Can impact all 4 of the "Grand Challenges" outlined in the recent DOE x-ray optics workshop thin-film chapter
  - R&D on film damage origins, mitigation, and lifetime
  - Experimental verification of film growth computational modeling
  - Development of methods for true 3-D film thickness gradients
  - MLL R&D on larger apertures and materials for expanded energy range



# Optics roadmap

- Where in 3 years?
  - Delivery of improved crystal optics and optical systems for high resolution analyzers (<10 meV, high throughput; plus sub-meV) and for high-heat-load monochromators.
  - Profiled deposition to give old beamline mirrors new life with dramatically improved figure and finish.
  - Partnership with other institutions on compound refractive lenses, and mirror and multilayer substrates.
  - Pathway towards energy tunable sub-20 nm nanofocusing up to 25 keV using stacked zone plates.
  - Pathway towards sub-10 nm nanofocusing at 25 keV using multilayer Laue lenses.
  - Begin revitalization of at-risk metrology and characterization systems.
  - R&D on improved thin film materials and growth strategies.
- Where with MBA Upgrade?
  - Delivery of sub-20 nm nanofocusing with tunability and easy alignment.
  - Optimized coherence-preserving beamline optics using simulations, profile deposition, and crystal optics fabrication.

# Optics: realizing the vision

- Investments being made from APS Operations, and APS Upgrade
  - 1-BM Optics and Detector test beamline
  - Simulation and modeling
  - Deposition systems
  - Crystal fabrication
  - Zone plate R&D towards production
  - Multilayer Laue lenses as best R&D path to sub-10 nm
- Need to renew at-risk metrology equipment
- Leveraging of Argonne resources: atomic layer deposition, nanofabrication at Center for Nanoscale Materials
- External proposals: DoE Accelerator and Detector R&D, National Science Foundation, SBIR (e.g., Advanced Diamond Technologies)

# Detectors: Where are we now?

- Detector Pool
  - Operational efficiency: detectors for specific beamline experiments, with technical support.
  - Outlet to introduce new, cutting-edge commercial detectors to the entire APS community (e.g., GE a-Si flat panels, Vortex ME-4, Pilatus, Pixirad CdTe, Eiger)
  - Detector characterization at new Optics and Detector Test beamline (1-B): support internal research and development, and attract outside groups for testing (e.g., XFEL's AGIPD).
- Detector Electronics
  - Expertise in analog and digital electronics for detector-related needs (high speed timing and synchronization, V-to-F)
  - Data acquisition systems (custom hardware and software), such as Platinum, FastCCD (LBL/ANL).
- Detector R&D
  - Superconducting energy-dispersive detectors: MKIDs
  - Pixel array detectors: FASPAX plans
  - SBIR collaborations (Agiltron, RMD, Voxtel)

# Detector Pool roadmap

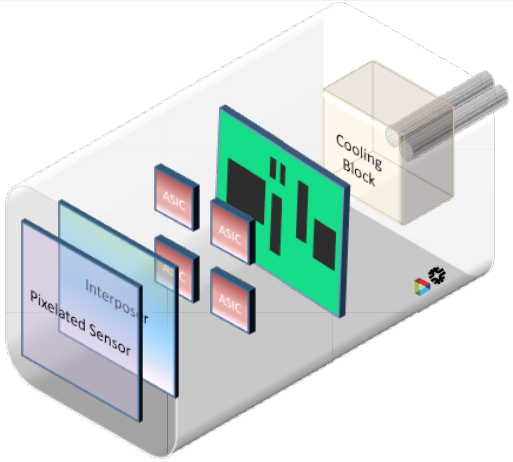
- Continue to bring in cutting-edge detectors for testing.
  - Mixed-mode PAD from ADSC/Cornell.
  - Detectors from the medical imaging market (e.g., flat panel CMOS, CdTe).
  - Testing of new detectors without interrupting operations at other XSD beamlines.
- Automated scintillator/optics characterization system at 1-BM
- Work with industrial or national lab partners on detector system development:
  - Wide field-of-view and high-resolution optics for tomography and near-field diffractive imaging?
  - Silicon Drift Diode arrays for x-ray fluorescence (e.g., BNL/CSIRO MAIA, or commercial vendors)?
  - Example funding source: SBIR

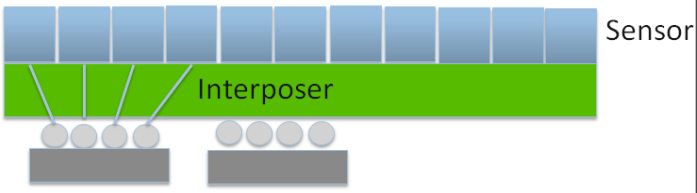
# Detector R&D: Energy-dispersive superconductors

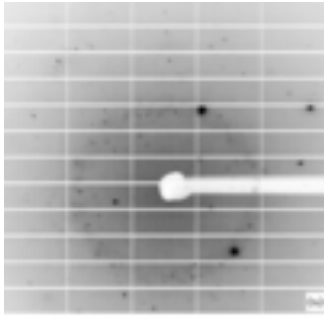
- Motivation
  - Single-eV resolution over wide energy range could make possible rapid spectroscopic imaging at nanoprobes, as well as impact on RSXS (29-ID), XAS, XES, ED-XRD, Compton scattering.
- Where are we now?
  - Exploring microwave kinetic inductance devices (MKIDs) as sensor, or as readout electronics for transition edge sensors (TES).
  - Year 4 of 5-year Early Career award.
  - Synergy with efforts in MSD/HEP; core component of a possible ANL "Detector Center" with dedicated clean room space and fabrication facilities.
  - Joint funding proposal to DoE/SUF from APS, NIST (J. Ullom), and Stanford/SLAC (K. Irwin)?
- Where in 3 years?
  - 1000-pixel prototype detector for demonstration experiments at the APS.
  - R&D on improvements including energy resolution and active fractional area.
- Where with MBA Upgrade?
  - 2000-pixel facility detector taking science data.

# Detector R&D: fast pixel array

- Fermi-Argonne Semiconductor Pixel Array X-ray detector (FASPAX):
  - 13 MHz burst frame rates; in-pixel analog storage
  - Novel integrating circuit for high dynamic range
    - $10^5$ x-rays/pulse on single 100 µm pixel
    - 3 stage gain
  - Unique gap-less sensor; interposer to ASICs
  - Intended uses:
    - High resolution movies for time resolved applications
    - Irreversible processes: Pump-probe-probe-probe
- Ptychography/Bragg CDI variant:
  - High dynamic range detector with small pixels (50-60 µm) optimized for coherence-based science
  - Shares many systems with FASPAX for cost-effective development
- Both implement features for enabling new science with MBA lattice upgrade.



T. Weber *et al.*, *Appl. Cryst.* **4**, 669-674 (2008).

# Detector R&D: fast pixel array plan

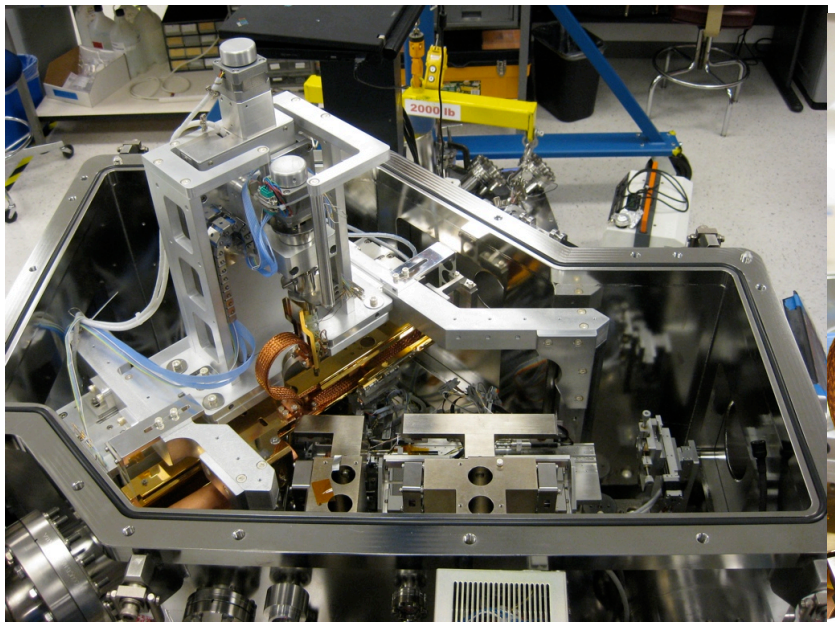
- Today:
  - Developing an R&D plan with the APS-Upgrade
  - Collaborating with Fermilab
- In 3 years:
  - Working prototypes of sensor, ASIC, and interposer assembly
  - X-ray testing and detailed characterization of assemblies
  - Complete final designs and plans to produce final detectors for the APS Upgrade
- At MBA Upgrade:
  - Delivery of Mega-pixel scale detectors for APS beamlines
  - Development of standard infrastructure (readout boards, data acquisition system, software) which can be applied to other area detector needs

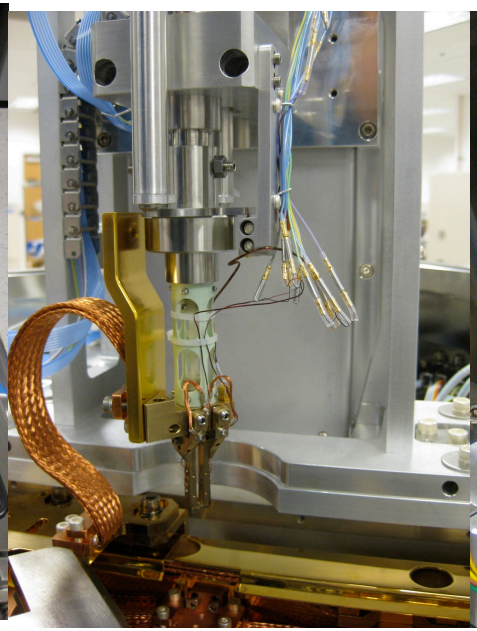
# *In situ* environments

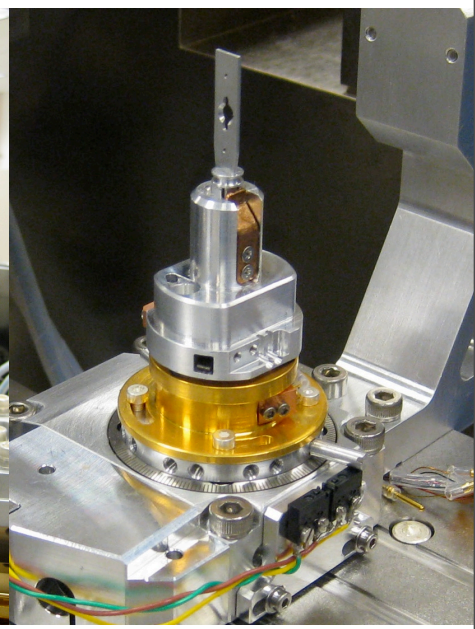
- Like with Big Data, there is no formal group tasked with this.
- But APS motto: "Real materials in real time under real conditions."
- Current developments:
  - Diamond anvil cells for high pressure research.
  - Magnetic fields.
  - Argonne Multi-Purpose *In Situ* X-ray (AMPIX) cell for electrochemical energy storage materials.
  - Small cell for fluid flow, temperature control on nanopositioning stages: SBIR with Hummingbird Scientific
  - R&D on nanopositioning:
    - Flexure-based systems with high precision and stability.
    - Control systems using feed-forward approaches instead of standard PID (proportional, integral, derivative) feedback.

# *In situ* at cryogenic conditions

- Standard for hard materials, macromolecular crystallography.
- Soft and bio materials for microscopy (nanopositioning):
  - Cryo Sample Preparation Lab (438-E030; NIH R01) with high pressure freezer, cryo ultramicrotome, cryo light microscope.
  - Cryojet option developed for x-ray microprobes.
  - Cryo sample exchange system: Bionanoprobe (Northwestern, Xradia/Zeiss, LS-CAT, XSD).





# *In situ* environments: future plans

- In 3 years:
  - Leader in correlative, multiscale imaging of real materials in real conditions - what hard x-rays are best at!
- With MBA Upgrade:
  - Proposal for *In Situ* Nanoprobe beamline
  - Sub-5 K Nanoprobe?
  - Environments for *in situ* studies throughout the APS
- How to get there?
  - R&D within XSD
  - Imaging Initiative LDRD
  - SBIR and other external partnerships
  - Focused team on high end instrumentation development?

# Overall comments

- The APS has strengthening efforts in big data, optics, detectors, and *in situ* environments.
- Initiative is coming from XSD - but APS lacks...
  - Concentrated high-end engineering team for developing sophisticated instrumentation.
  - Concentrated high-end computing team implementing next-generation technologies.
- There are other models for computing and instrumentation:
  - Oak Ridge has a Neutron Data Analysis and Visualization Division led by a neutron scientist (Thomas Proffen).
    - Groups: Technology Advancement (HPC systems and data infrastructure), Scientific Data Analysis Group, Instrument Data Aquisition and Controls, Control Systems.
    - Center for Accelerating Materials Modeling.
  - ESRF has a Instrument Services and Development Division led by a x-ray scientist (Jean Susini)
    - Separate from the Technical Infrastructure Division.
    - Project funding is allocated by Experiments Division.

# Thanks to many!

- Including many not pictured here!