Argonne
NATIONAL LABORATORY

... for a brighter future

Turbocharging XPCS at 8-ID: Focusing, FPGA's and Fast Computing

Alec Sandy

X-Ray Science Division

Argonne National Laboratory

APS User Operations Meeting: May 20, 2009

U.S. Department of Energy

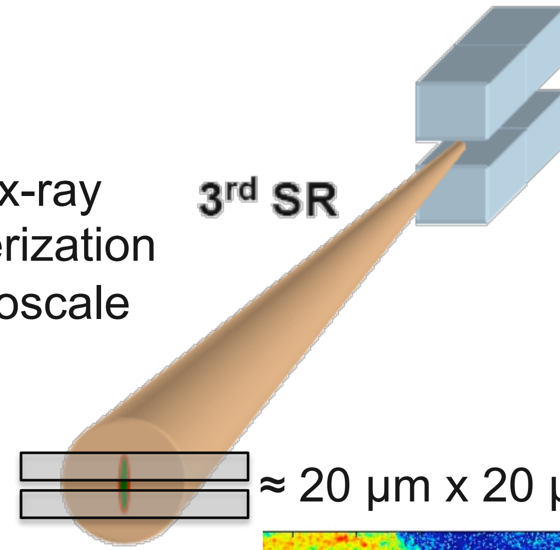
UChicago Argonne LLC

Office of Science
U.S. DEPARTMENT OF ENERGY

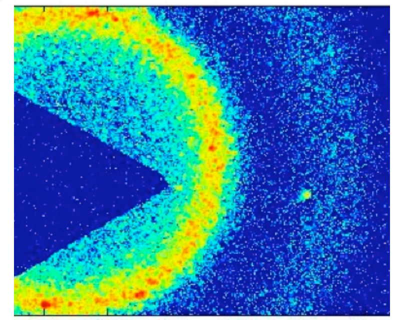
A U.S. Department of Energy laboratory managed by UChicago Argonne, LLC

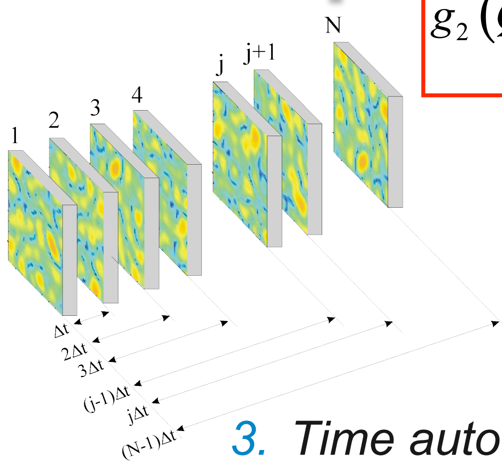
Introduction

- X-ray photon correlation spectroscopy (XPCS) is the x-ray analog of dynamic light scattering permitting characterization of the slow dynamics of condensed matter at the nanoscale
  - Experiment mechanics
    1. *Illuminate disordered sample with a (partially) coherent x-ray beam*
    2. *Collect speckle pattern versus time with a high resolution and high gain area detector*

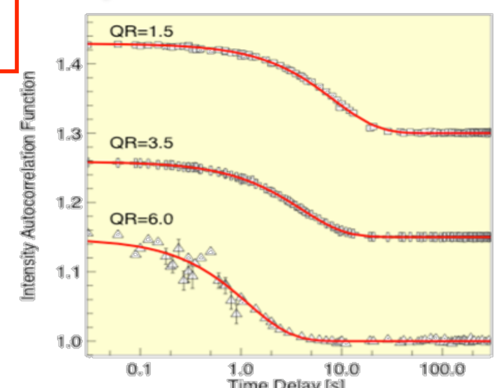


≈ 20 µm x 20 µm





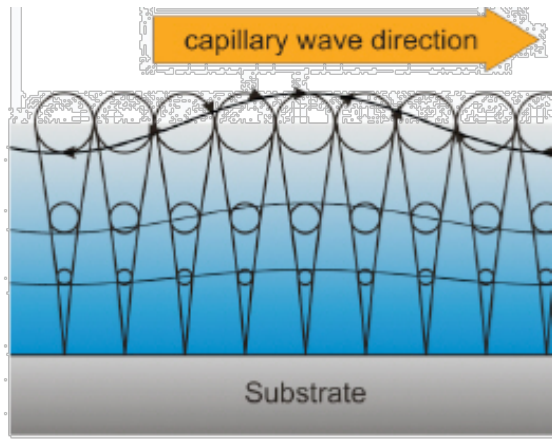
$$g_2(Q,\tau) \equiv \frac{\langle I(Q,t)I(Q,t+\tau)\rangle}{\langle I\rangle^2}$$

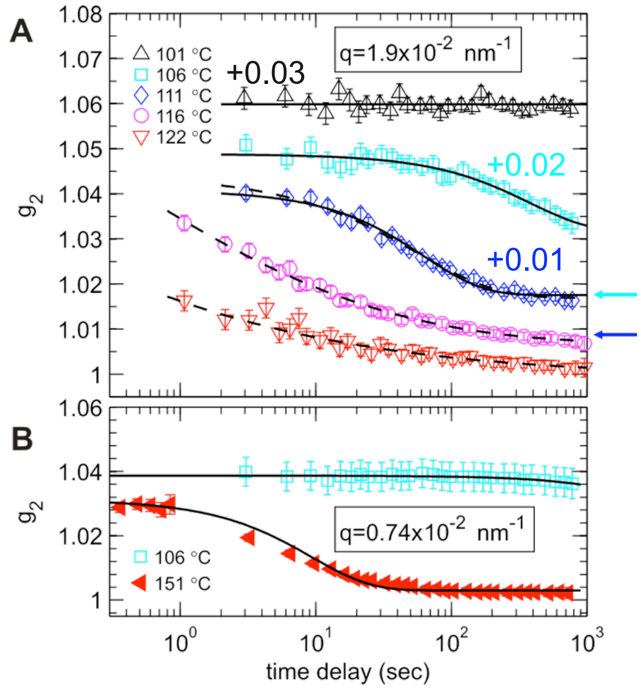


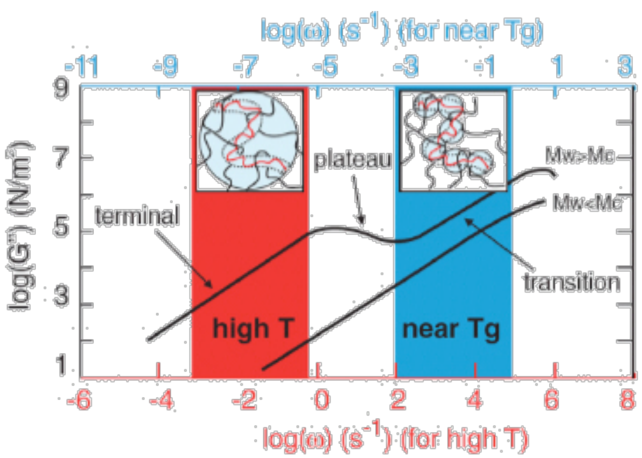
3. *Time autocorrelate fluctuating speckle pattern to reveal sample dynamics*

Introduction

- Many recent examples of good XPCS-related science from 8-ID …
  - Polymer film dynamics near the glass transition
    - *Distinguish between dynamics of entire polymer chains and dynamics between entanglements of polymer chains*







*Z. Jiang, M. Mukhopadhyay, S. Song, S. Narayanan, L.B. Lurio, H. Kim, and S.K. Sinha, PRL **101**, 246104 (2008)*

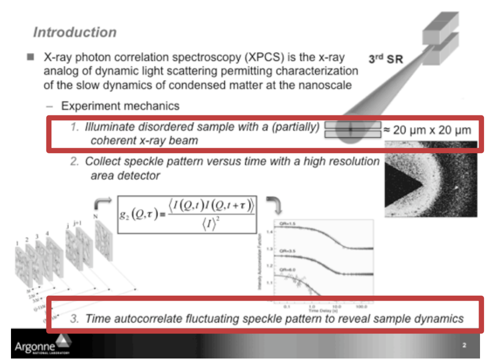
Introduction

- Key technical elements in 8-ID's success have been:
  - Preserving the coherence of the x-ray beam delivered to the sample
  - Applying high-gain, small-pixel area detectors to XPCS
    - *Allows complex dynamic behavior to be simultaneously probed over many length scales and decades in delay time (multi-speckle XPCS)*

So what could be better?

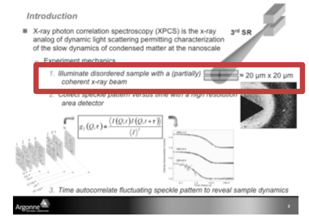
1. Coherent flux utilization ➔ vertical focusing

3. Effective use of fast area detectors

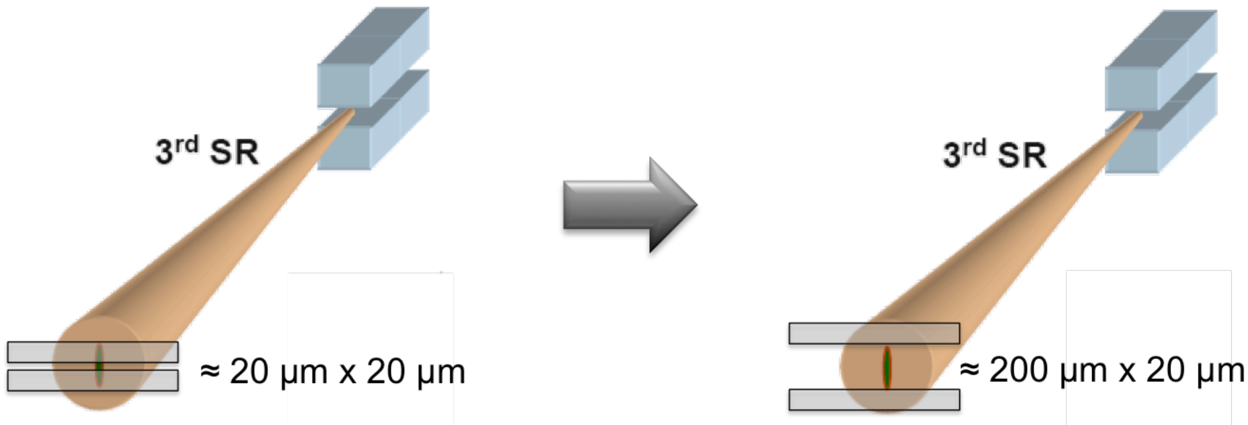

Introduction

- X-ray photon correlation spectroscopy (XPCS) is the x-ray analog of dynamic light scattering permitting characterization of the slow dynamics of condensed matter at the nanoscale
  - Experiment mechanics
    1. *Illuminate disordered sample with a (partially) coherent x-ray beam*
    2. *Collect speckle pattern versus time with a high resolution area detector*
    3. *Time autocorrelate fluctuating speckle pattern to reveal sample dynamics*

Vertical Focusing



1. Only 10% of coherent flux supplied by the APS is used (far-field diffraction limit)

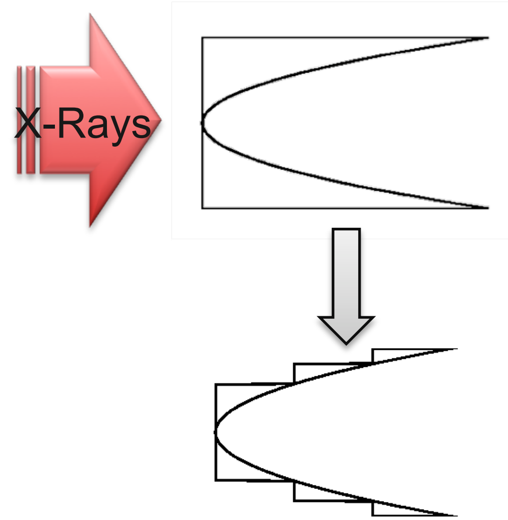


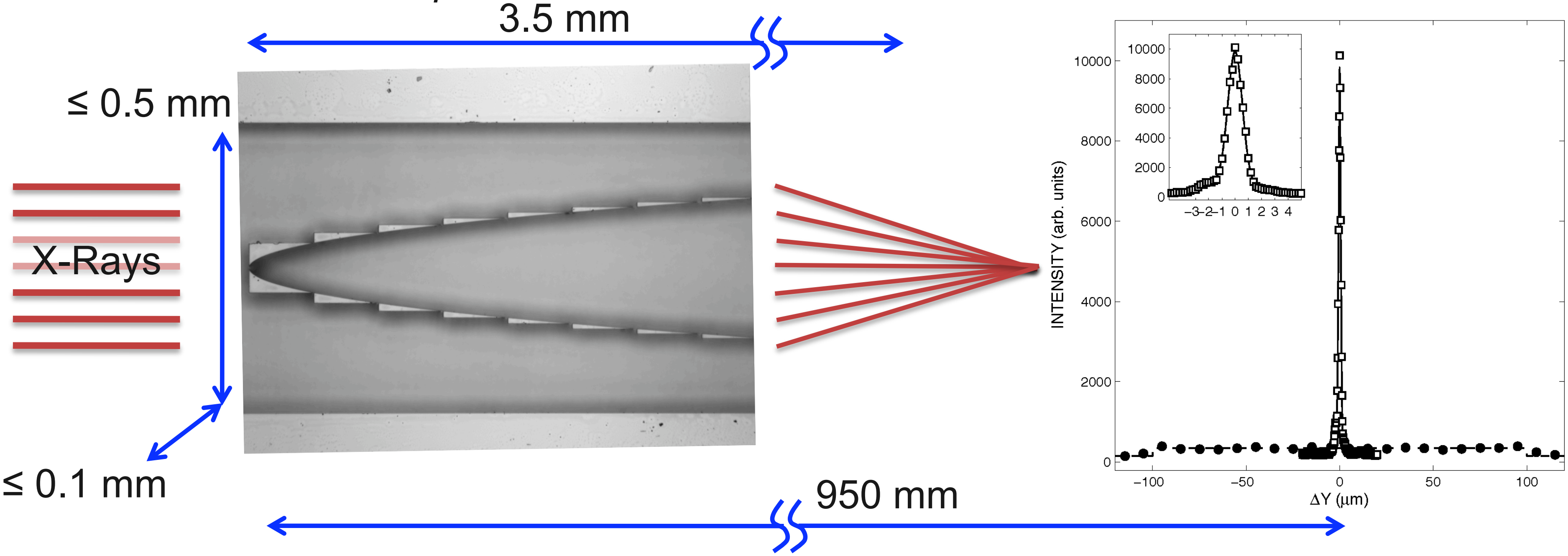
- Implement brilliance preserving vertical focusing so that the entire coherent flux delivered by the APS is used

- Beamline 8-ID focusing options are constrained
  - Preserve well-collimated unfocused beam for upstream “end” station
  - Only moderate demagnification and “clean” beam (SAXS geometry)
  - Reshaped beam rather than a small beam so high efficiency is required
  - Limited budget for exploratory project

Vertical Focusing

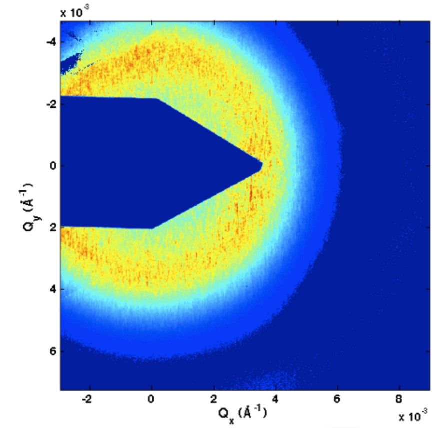
- (A) Solution: silicon kinoform lenses
  - Refractive optic … absorbing material removed
    - *“Ideal” blazed zone plate … but 1-D only*
  - Kinoform focusing performance
    - *Efficiency ≈ 45%*
    - *Gain = 28x*
    - *FWHM ~ 1.3 µm*



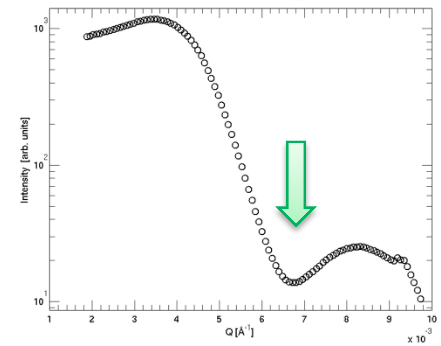


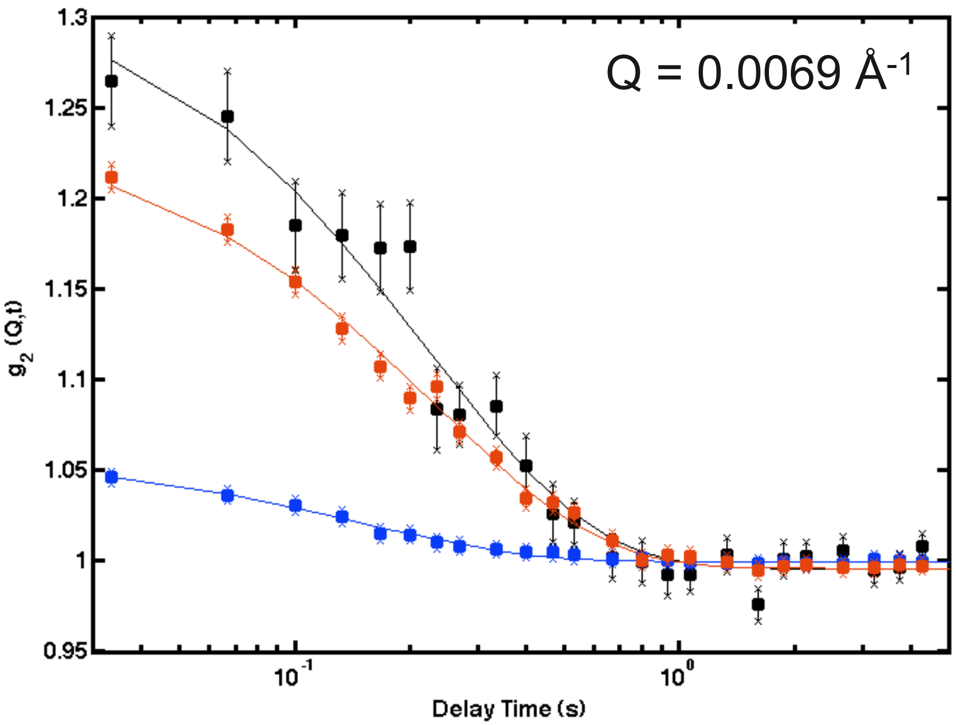
Vertical Focusing

- Kinoform performance vis-à-vis XPCS
  - Dynamics of concentrated 70 nm radius latex spheres



- Lens provides ~ same coherence as smaller pinhole aperture but 5X more flux



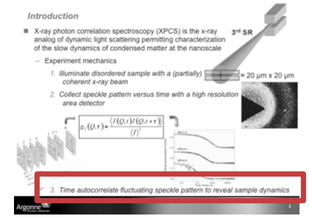


20 µm (V) X 20 µm (H) "pinhole", no lens, Intensity = 0.1

200 µm (V) X 20 µm (H) "pinhole", no lens, Intensity = 1

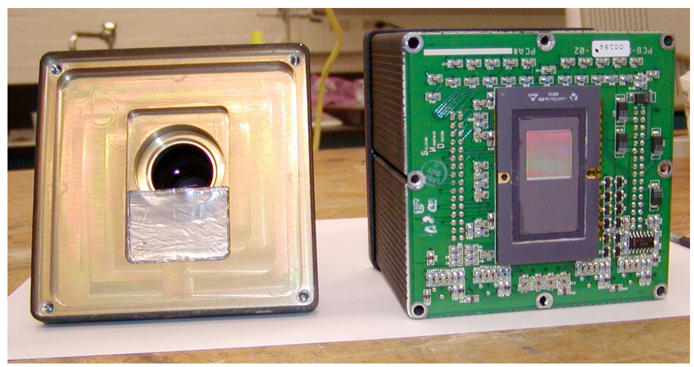
200 µm (V) X 20 µm (H) "pinhole", kinoform lens, Intensity = 0.5

Effective Use of Fast Area Detectors



3. Effective use of fast area detectors remain cumbersome
   - *Facile control of fast area detectors allows:*
     - EITHER a short series of images at fast frame rates OR a long series of images at slow frame rates

✔ *Pre-process (dark subtraction, compression, …) rapidly streaming area detector data via high-performance frame grabber with field programmable gate array (FPGA)*

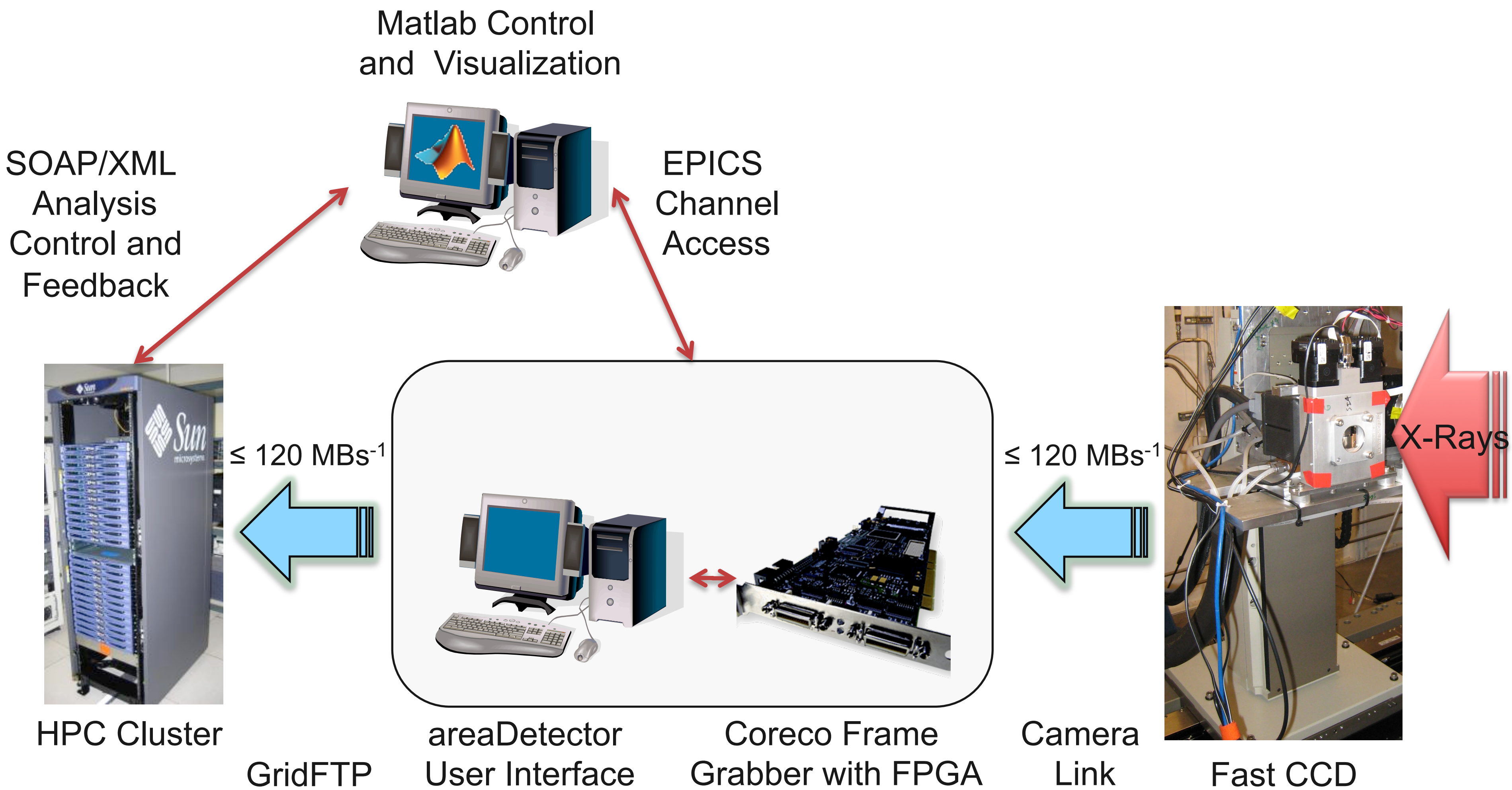


- *Ratio of data reduction time to data acquisition time has grown to unacceptable levels (1:1 ➔ 100:1)*

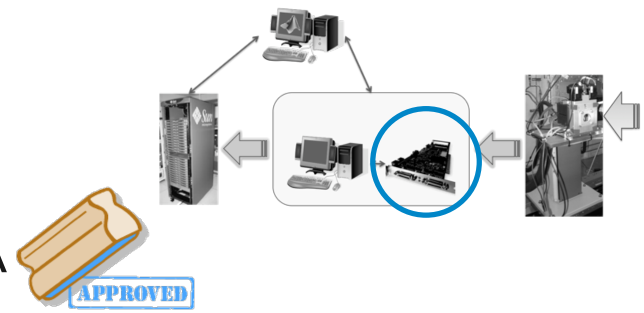
✔ *Rapid time autocorrelation via high-performance computing (HPC)*

Effective Use of Fast Area Detectors

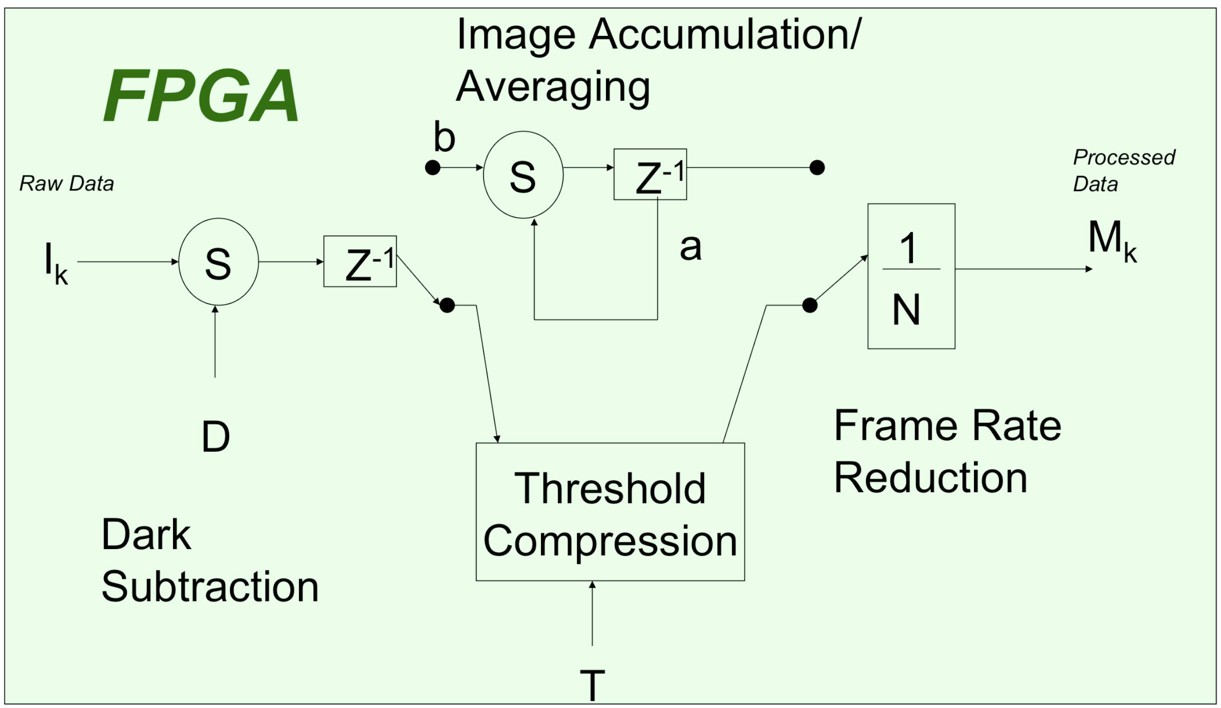
- System architecture and data flow



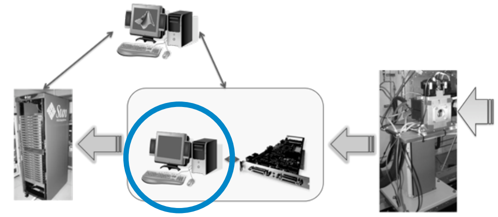
Effective Use of Fast Area Detectors



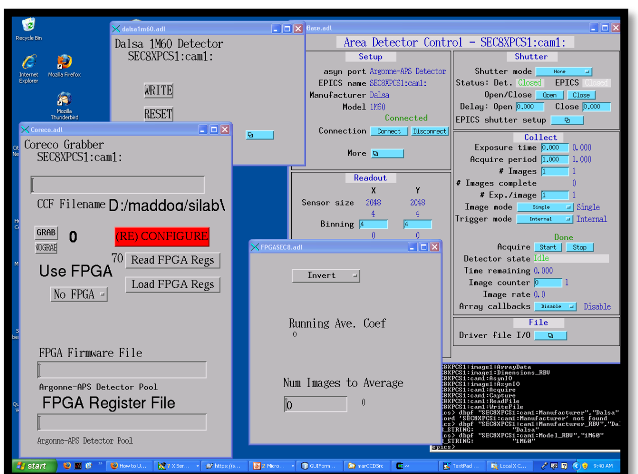
- Coreco Anaconda Frame Grabber
  - Officially-supported frame grabber of BCDA
  - 2 GB framebuffer
  - Xilinx Virtex-Pro FPGA with embedded CPU
  - On-the-fly averaging (dark), dark subtraction, thresholding, compression

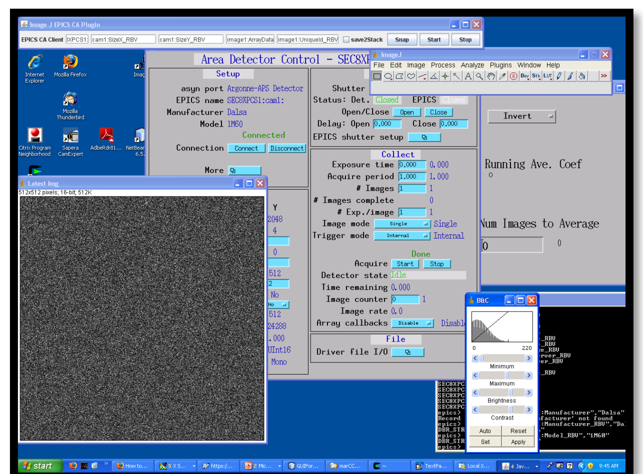


Effective Use of Fast Area Detectors

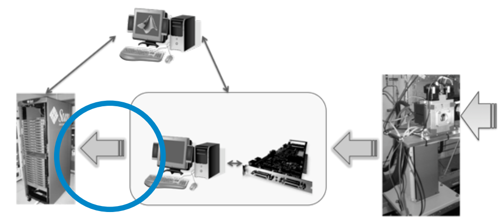


- Software developed for controlling FPGA and Dalsa/SMD CCD camera
  - Built using areaDetector, a relatively new EPICS software framework for controlling area detectors (Mark Rivers, CARS)
  - areaDetector implementation
    - *Controls functionality of FPGA*
    - *Controls functionality of CCD camera (frame grabber)*
    - *Functionality available via medm GUI and via other EPICS client applications such as 'spec,' 'Matlab,' …*

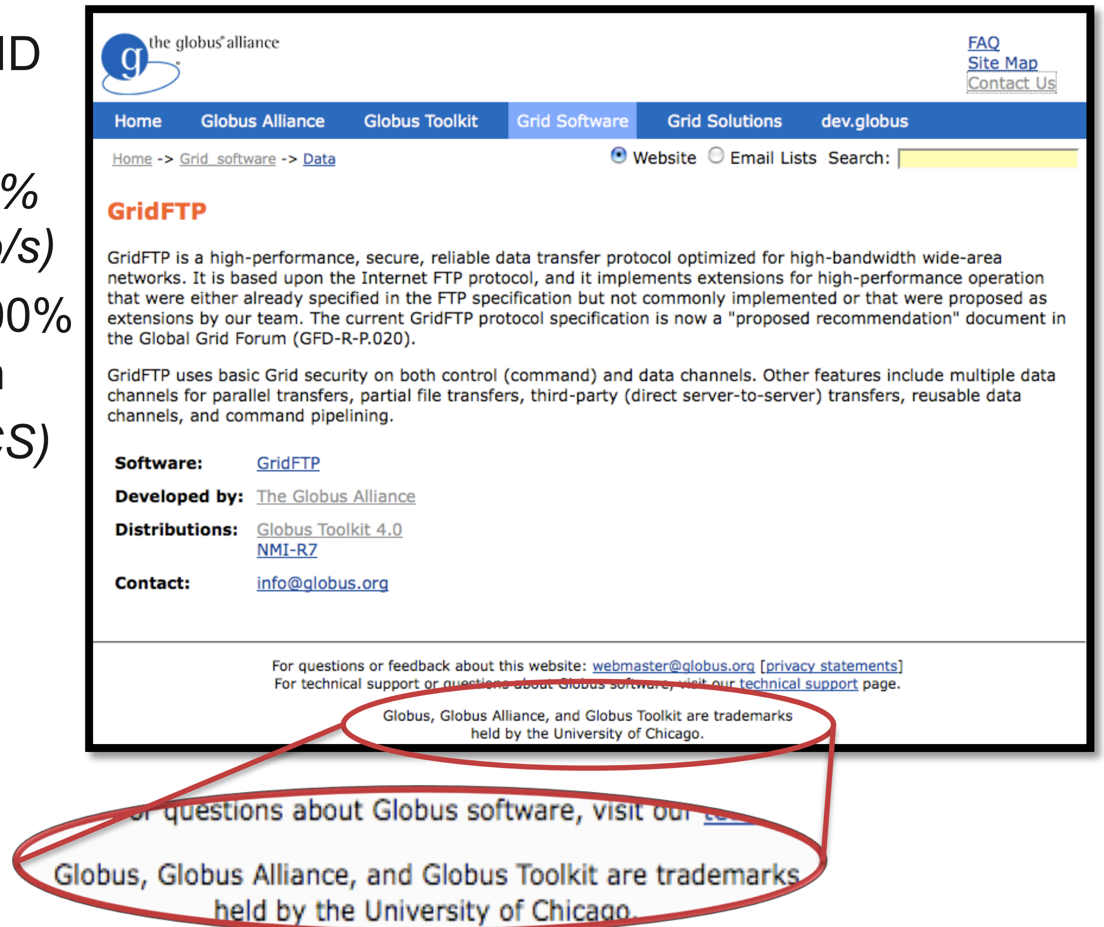




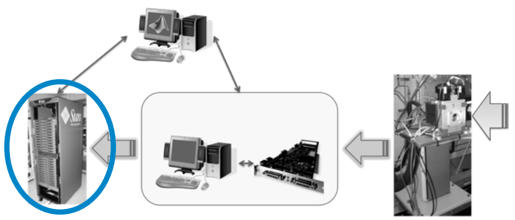
Effective Use of Fast Area Detectors



- GridFTP used to rapidly transfer data to PC-cluster for time autocorrelation
  - Data acquisition at beamline 8-ID
  - Cluster in APS data center
    - *“Normal” data transfers ~ 15% of available bandwidth (1Gb/s)*
  - GridFTP enables transfers ~ 100% of available network bandwidth
    - *Considerable local (ANL-MCS) expertise*
    - *Service callable from ‘spec’, ‘Matlab,’ …*



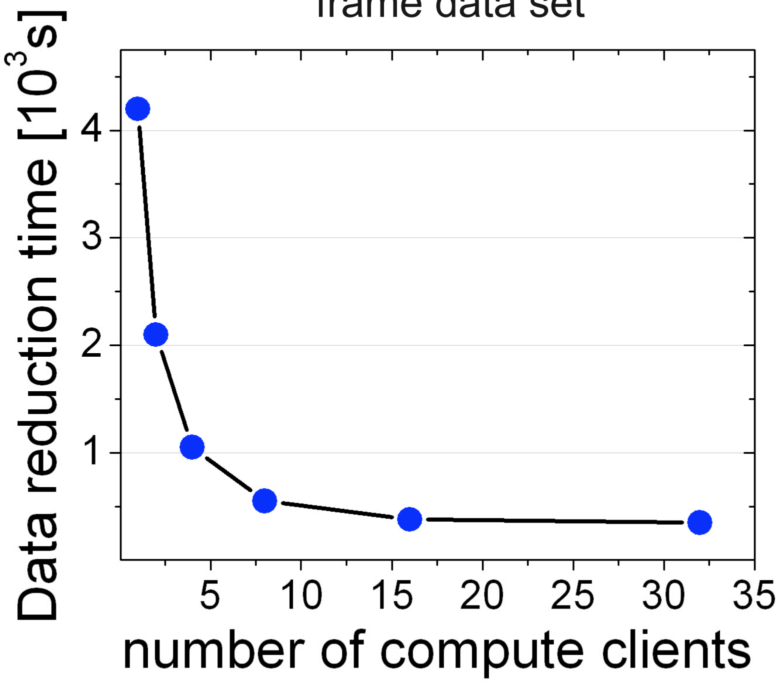
Effective Use of Fast Area Detectors



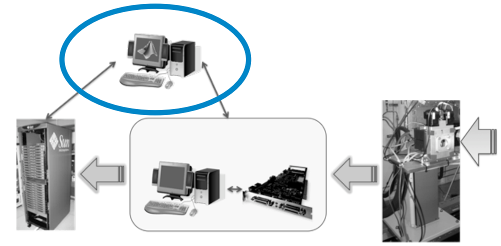
- XPCS multispeckle time autocorrelation is "embarrassingly parallel"
  - Time autocorrelations are done on a pixel-by-pixel basis and then binned appropriately at the end

- Parallelized version of time autocorrelation code developed and extensively tested on APS development and production clusters
  - 10,000 1,024 X 1,024 frames
    - *330 sec acquisition time (30 fps)*
    - *Time autocorrelation*
      - 1 CPU: > 4,000 seconds
      - 16 CPU's: < 400 seconds
  - Near real-time reduction possible

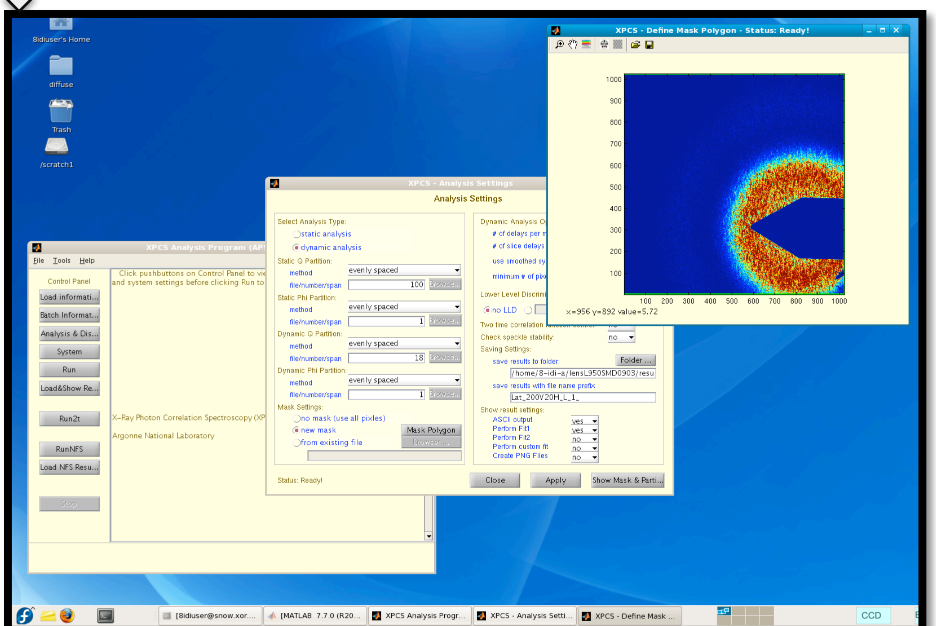
Results for a 1k x 1k x 10,000 frame data set

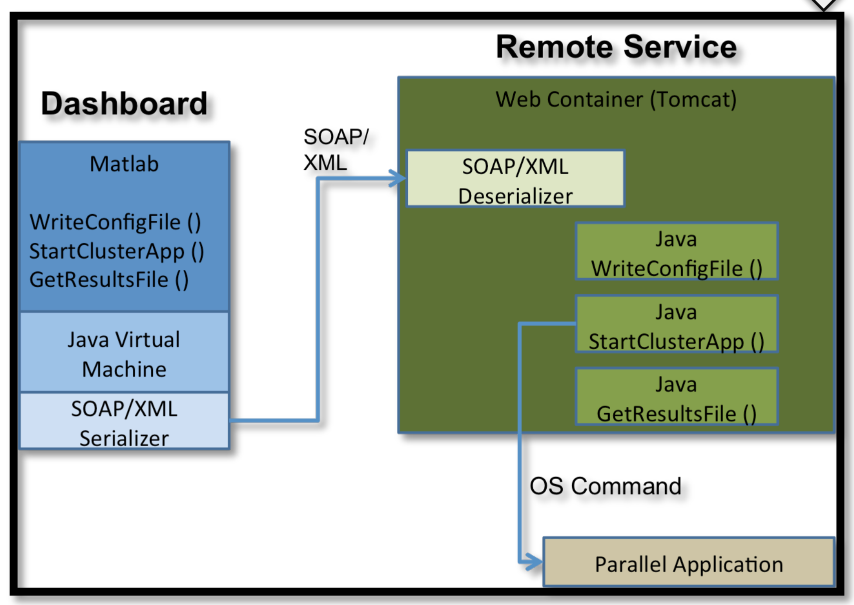


Effective Use of Fast Area Detectors



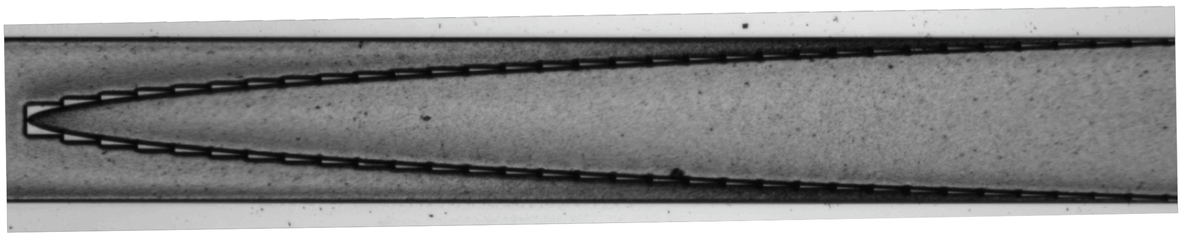
- Matlab used to create an overarching user-friendly interface to underlying hardware, firmware and software (Zhang Jiang)
  - EPICS channel access for camera/FPGA control
  - Java ➔ SOAP/XML calls for directing and monitoring cluster calculations
  - Time autocorrelations continue to be available locally in Matlab



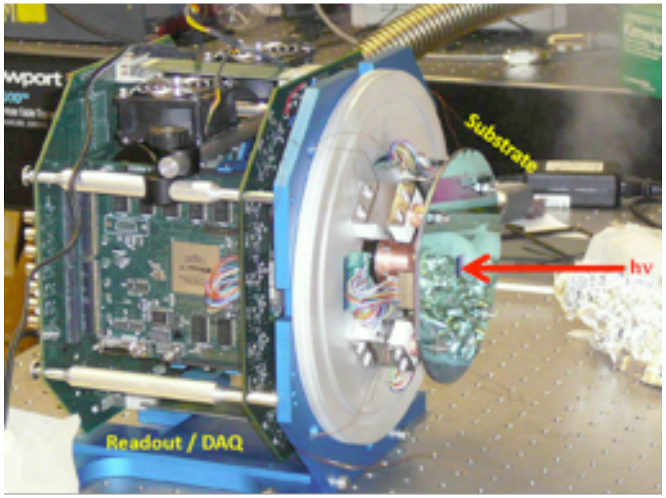


Conclusions and Future Directions

- Efficient vertical focusing used to increase coherent flux delivered to XPCS experiments at 8-ID-I by a factor of 5
  - Will deploy for select 8-ID-I experiments in 2009-2
  - Significantly increased signal-to-noise or access to faster time scales
  - Supply of kinoform lenses needs to be improved
    - *Beryllium compound refractive lenses are a possible future alternative*



- FPGA and HPC nearly ready to provide near real-time autocorrelation of speckle patterns
  - Pilot for select experiments during 2009-2 cycle at 8-ID-I
  - Extend infrastructure to ANL-LBL Fast CCD



Acknowledgements

- Focusing
  - XSD-XOR
    - *Jun-Dar Su and Suresh Narayanan*
      - Experiments and data processing
  - BNL NSLS and CFN
    - *Abdel Isakovic and Ken Evans-Lutterodt*
      - Kinoform lens fabrication
- Area detector work
  - XSD-XOR
    - *Marcin Sikorski (strategic LDRD), Suresh Narayanan (and Michael Sprung)*
      - Science applications, Matlab integration, proofing
  - XSD-BTS
    - *Tim Madden and John Weizeorick*
      - Frame grabber software (areaDetector) and FPGA firmware development
  - AES-BCDA
    - *Brian Tieman*
      - Parallelized code, GridFTP deployment, web services
  - Additional support from Pete Jemian (AES-BCDA) and Patricia Fernandez (XSD-BTS) and Dan Fraser and Rajkumar Kettimuthu (MCS)