

# Data Analysis and Management at the APS: Successes and Challenges

Nicholas Schwarz

Principal Computer Scientist / Group Leader

Software Services Group

APS Engineering Support Division

Advanced Photon Source

Argonne National Laboratory

15 August 2013

# APS Software Services Group

## Sprint Team



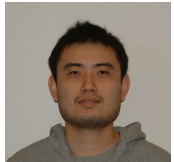
**Arthur Glowacki**  
*Software Engineering Specialist*



**John Hammonds**  
*Principal Application Developer*



**Faisal Khan**  
*Software Engineering Associate*



**Ke Yue**  
*Software Engineering Associate*

## APS-U



**Sinisa Veseli**  
*Principal Software Engineer*

## EPICS Team



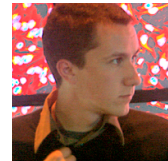
**Janet Anderson**  
*Computer Scientist*



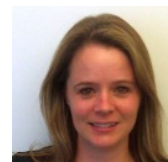
**Andrew Johnson**  
*Computer Scientist*



**Tim Mooney**  
*Physicist*



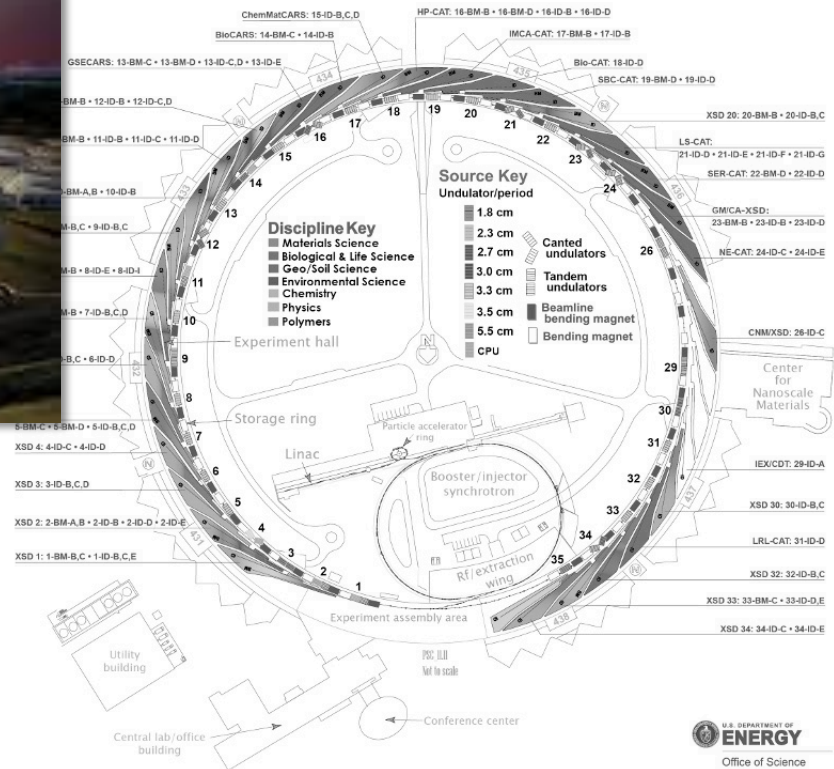
**Nicholas Schwarz**  
*Group Leader*



**Marianne Binetti**  
*Administrative Secretary*



# The Advanced Photon Source



# Increasing Amounts and Complexity of Data

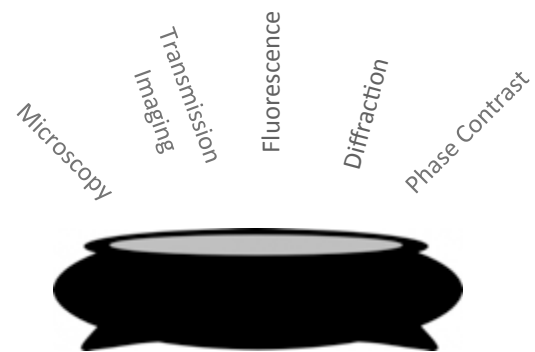
## Detectors



## Experiment Automation



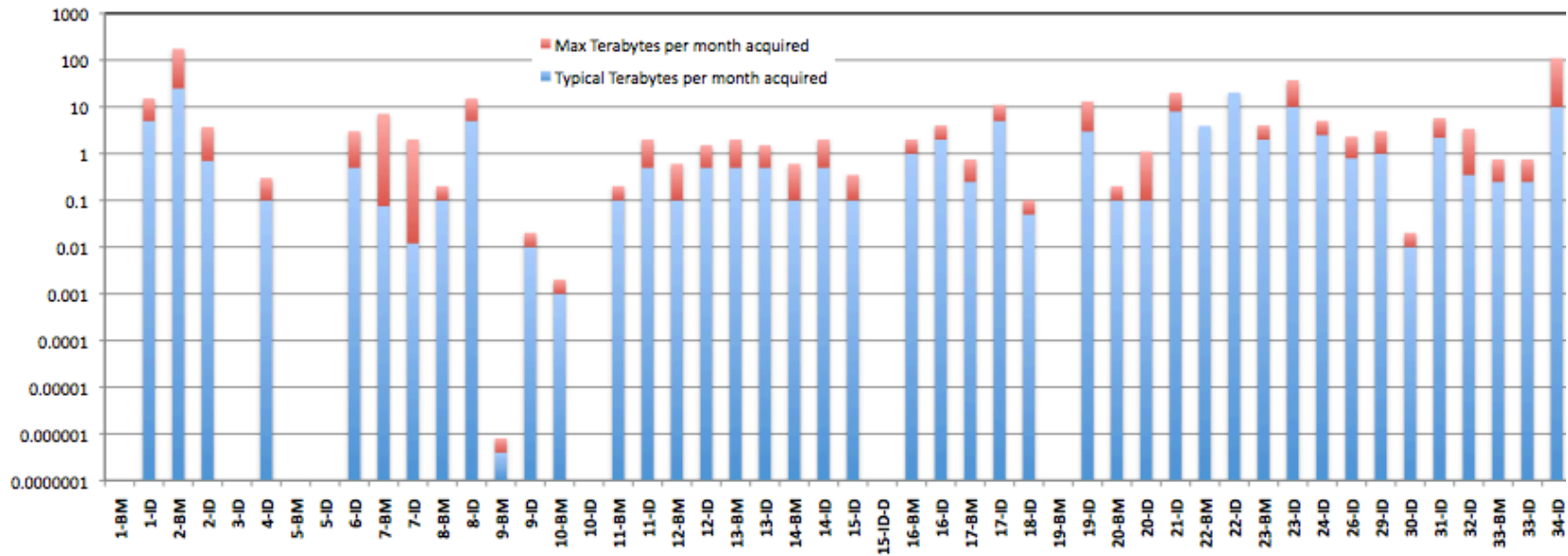
## Techniques





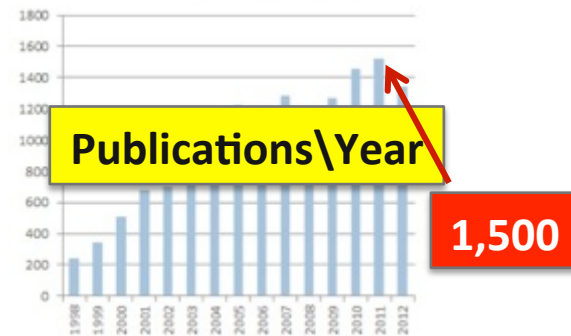
# APS Average Data Rate

Cumulative typical data volume at present: 112 TB/month  
 Cumulative maximum data volume: 368 TB/month

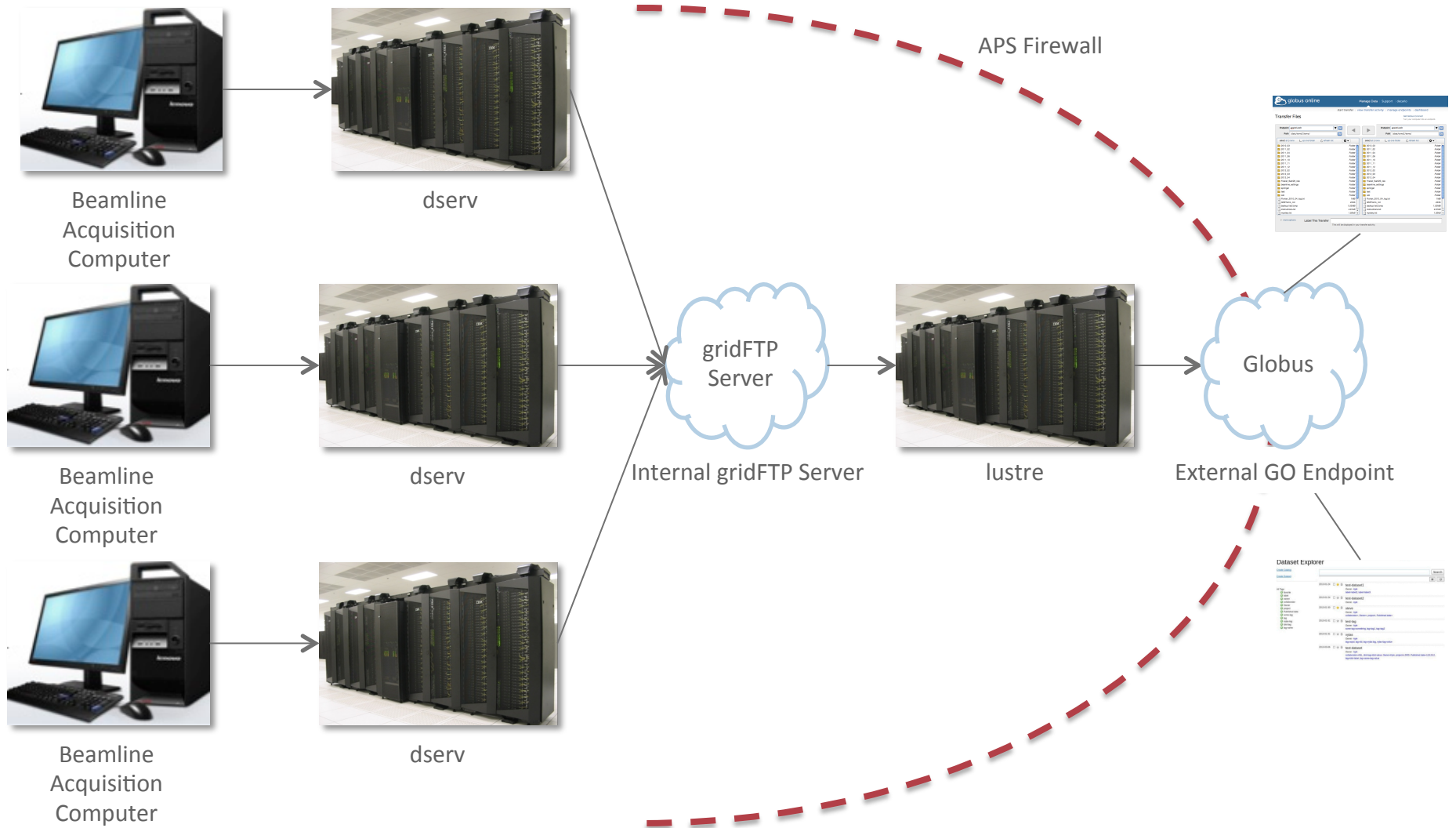


F. De Carlo (ANL)

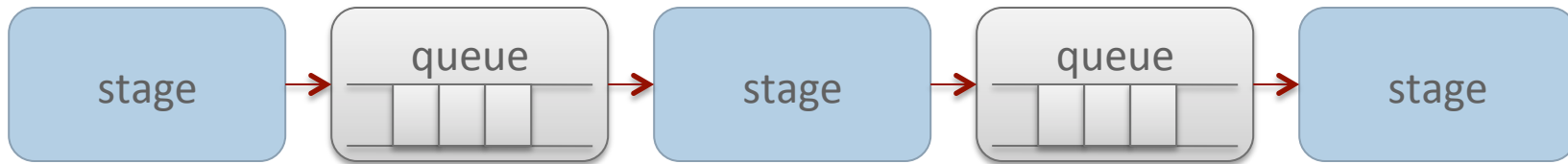
# Increasing User Base



# Architecture



# Workflow Pipeline

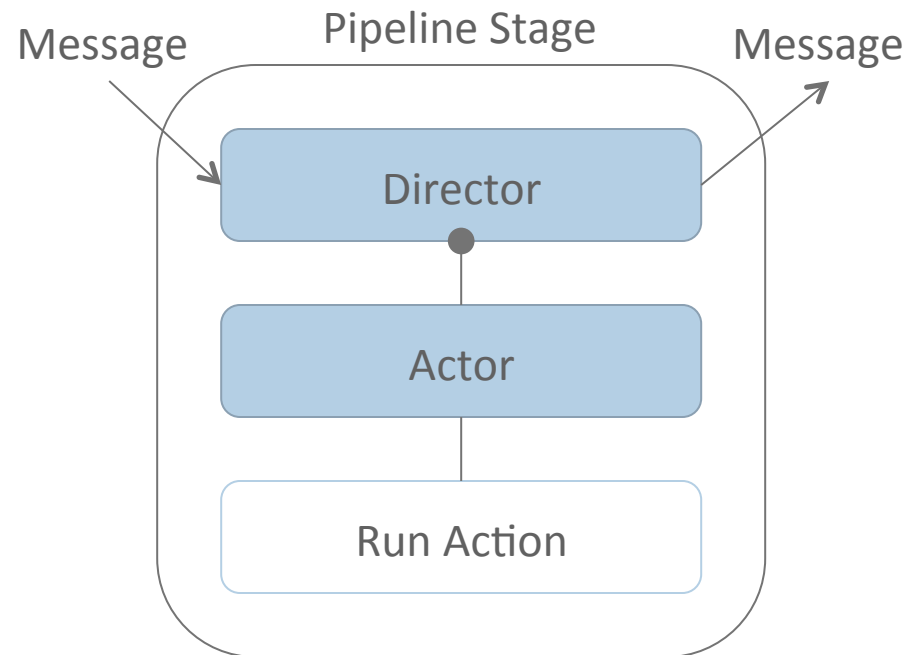


- Series of actors connected by message queues
- Stage
  - Acquisition
  - Run data analysis
  - Transfer files
  - Many languages: C++, Java, Python
- Message queues
  - Pass messages from one actor to the next
  - JMS message queues (ActiveMQ)

# Pipeline Stages

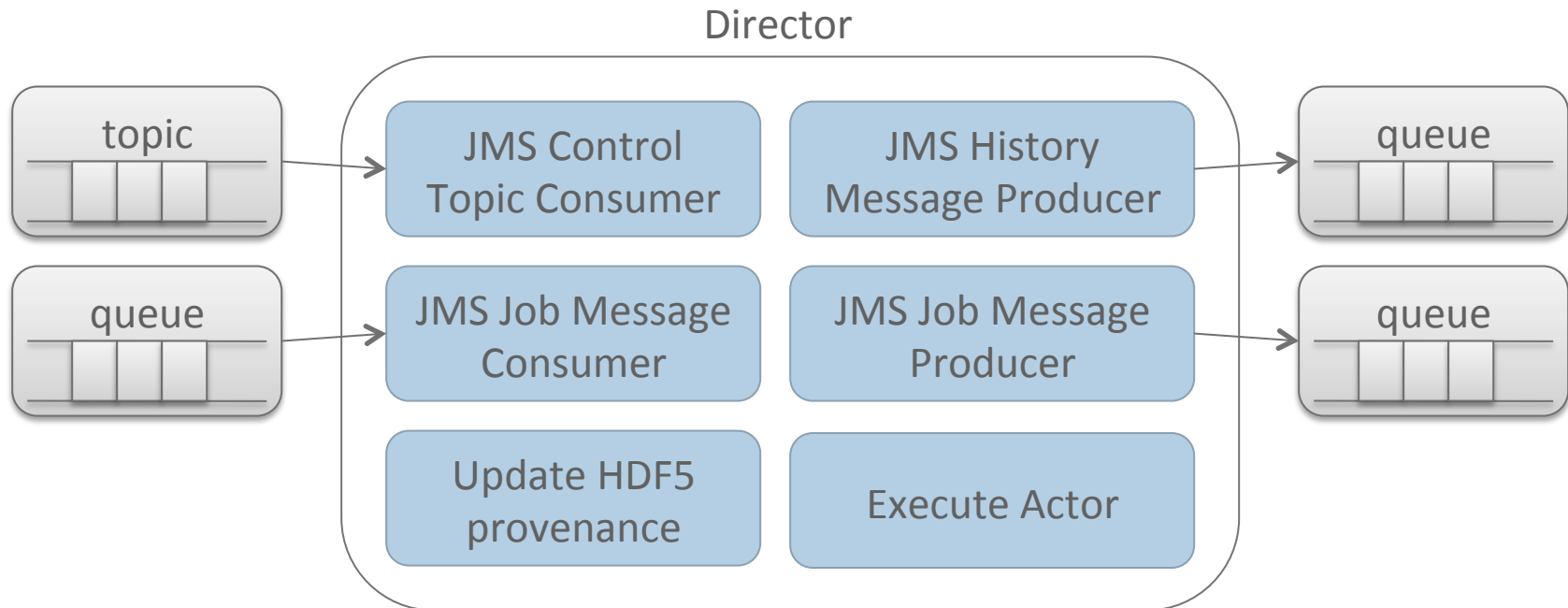
Stages are composed of two separate classes:

- Director
  - interface with the message broker
- Actor
  - run scan / analysis / file transfer
  - save results
  - report status





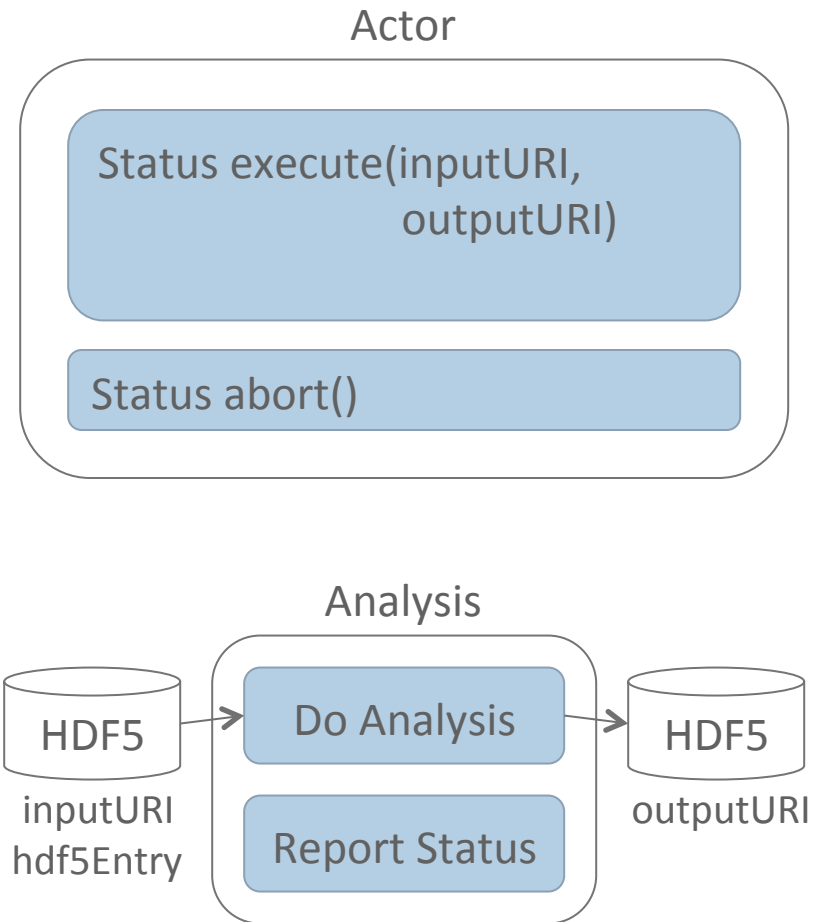
# Director



- Broker interface
- Handle job messages
- Control messages
- Update history
- Maintain provenance
- Execute Actor

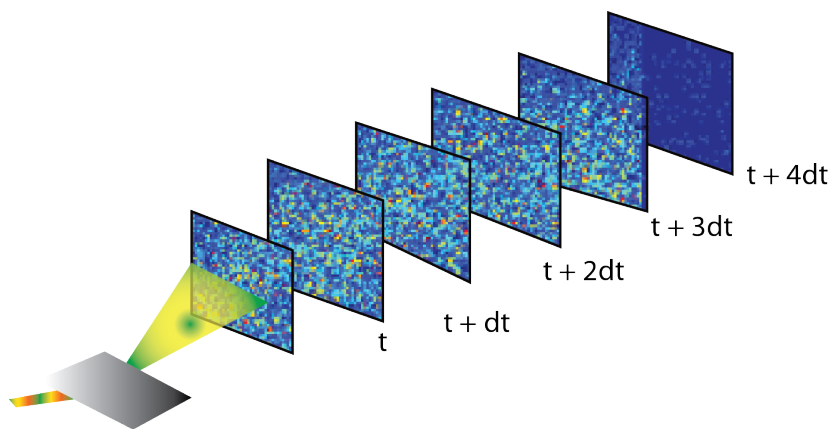
# Actor

- Actor
  - Called by Director
  - Abstract interface for concrete implementation
  - Execute job / analysis
  - Report status
  
- Analysis
  - External application
  - Internal code
  - Read input data from HDF5
  - Write output data to HDF5

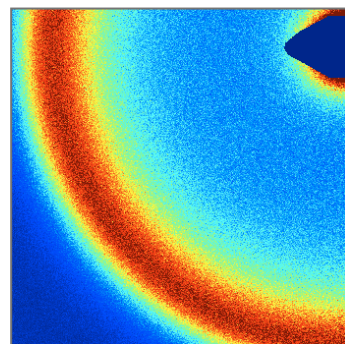
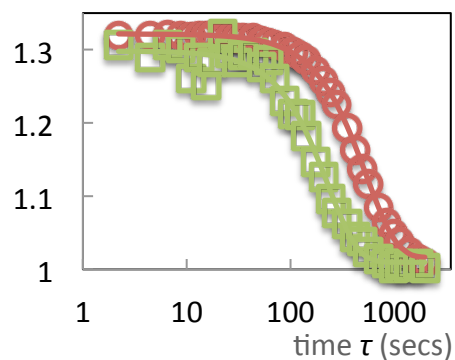


# X-ray Photon Correlation Spectroscopy (XPCS)

Suresh Narayanan and Alec Sandy (APS)



2D small-angle scattering pattern from a suspension of silica spheres (*right*).



$g_2$  calculation at two different length scales (*left*).

## Beamline and Detector

- 8-ID
- 1K x 1K @ 60 fps
- 1K x 1K @ 200 fps (FastCCD2)

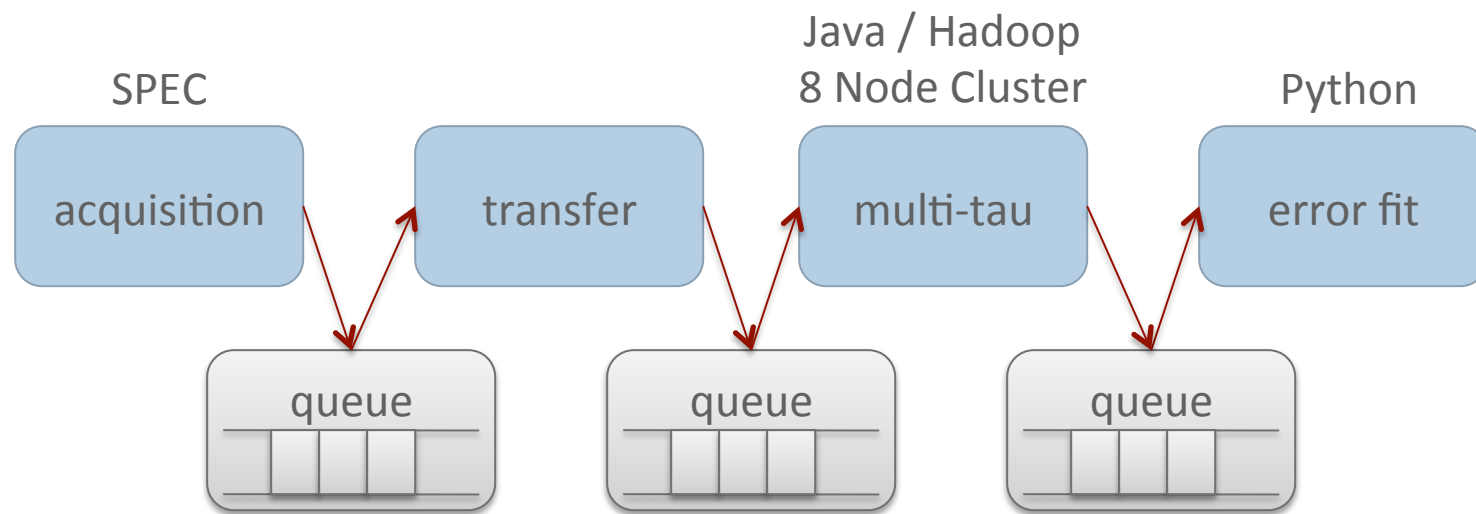
## XPCS Data

- Kinetics measurements
- 2D images over time
- A few minutes to collect
- Varies from 0.5 GB to 50 GB raw

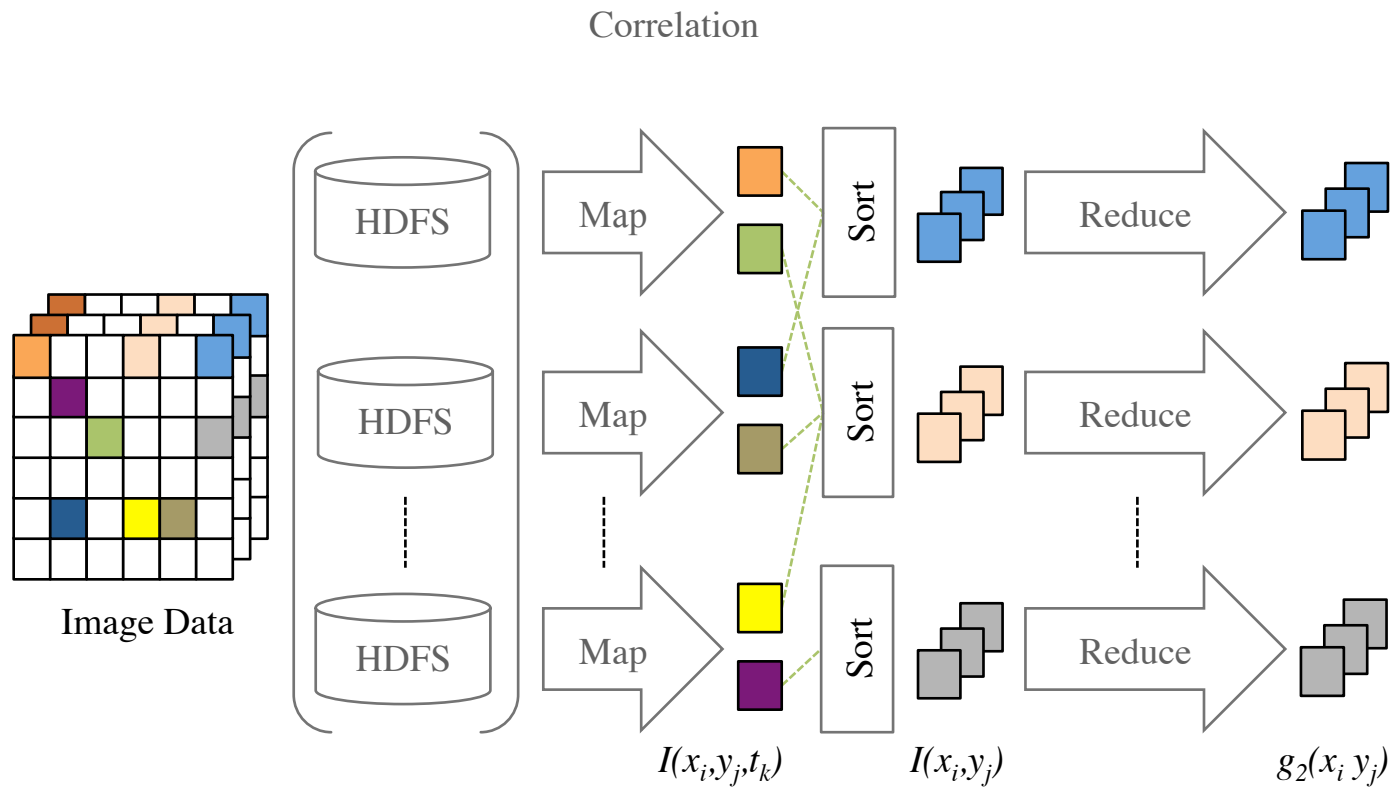
## Reduction

- Multi-tau autocorrelation

# XPCS - Data Workflow

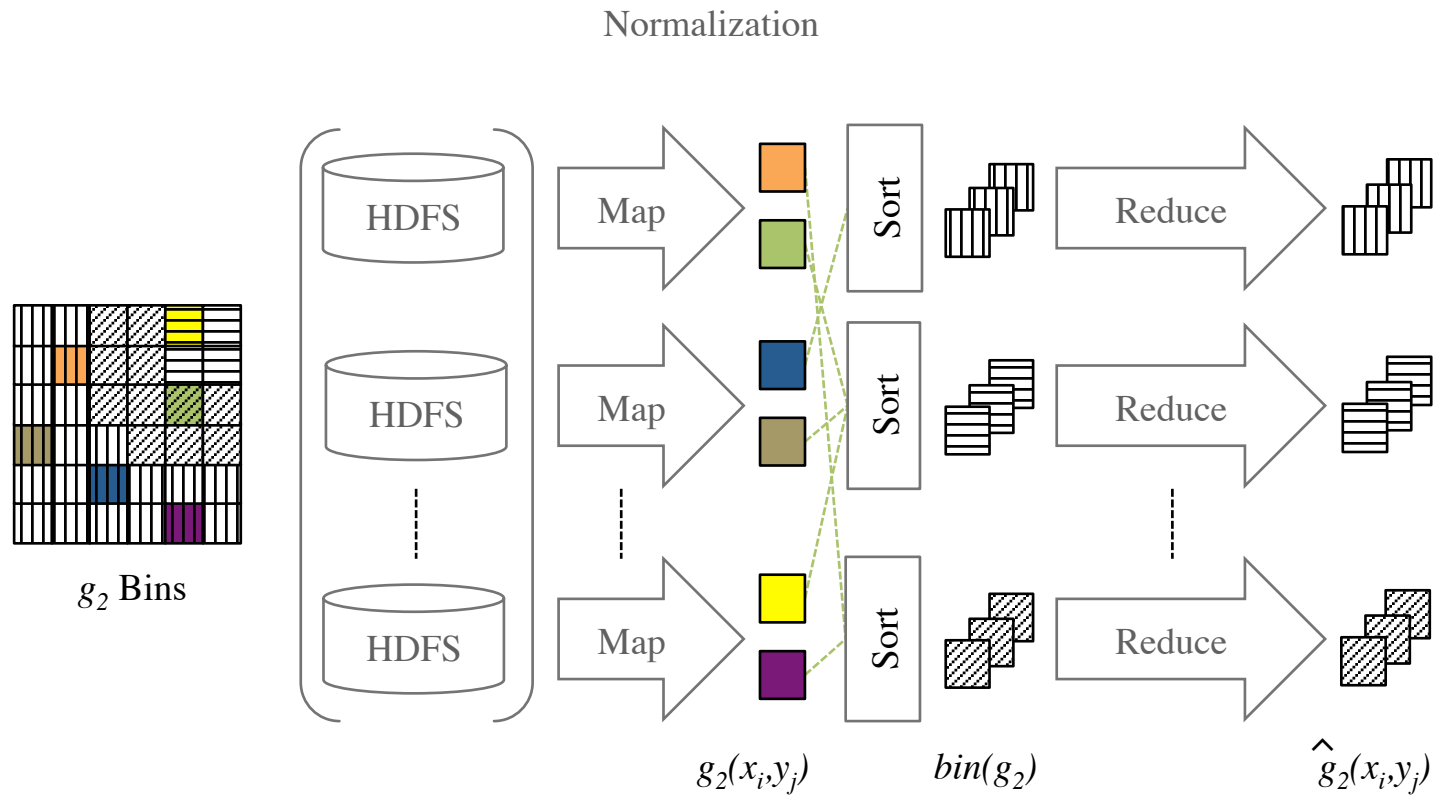


# XPCS - Hadoop Multi-Tau Autocorrelation





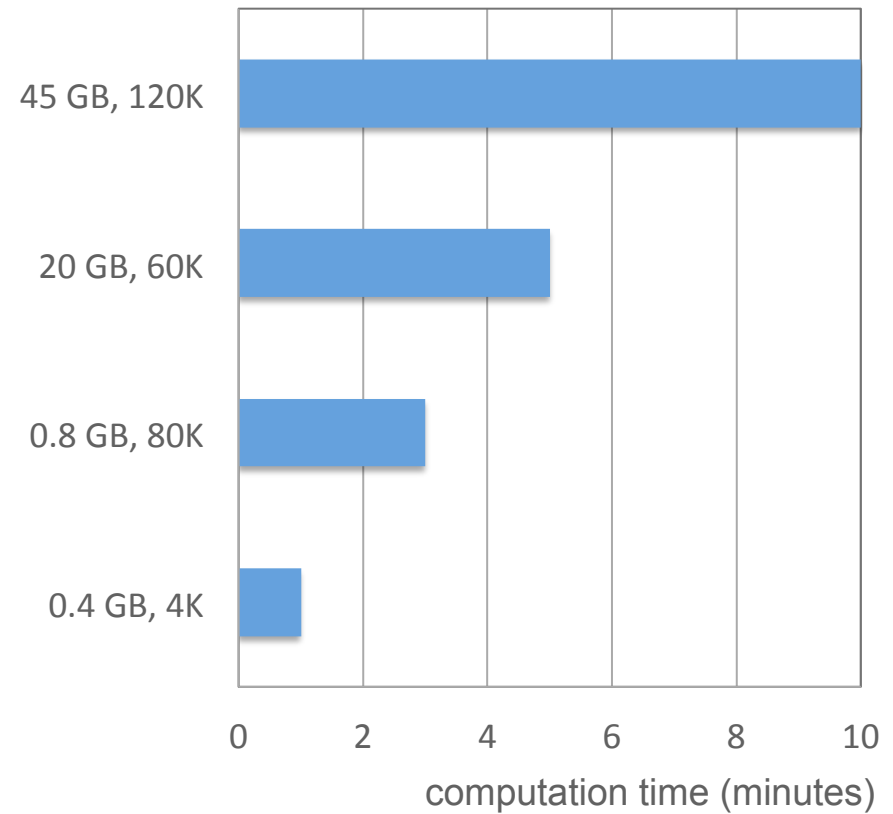
# XPCS - Hadoop Normalization



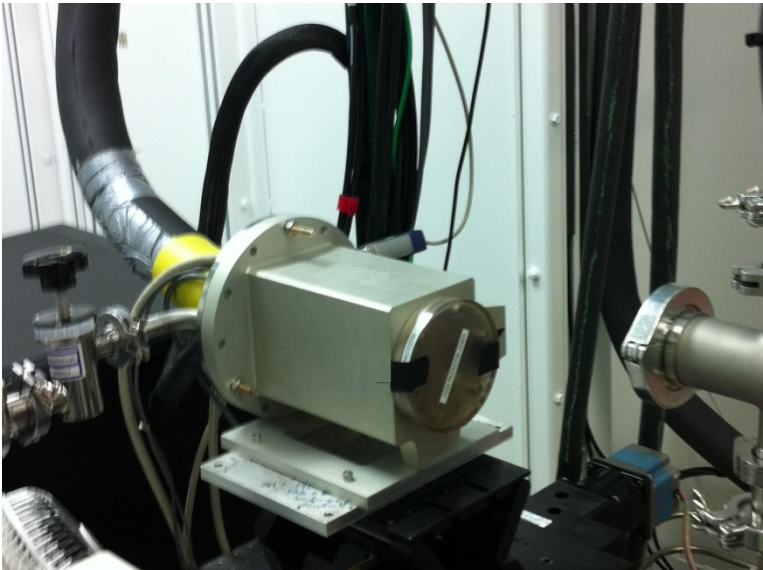
# XPCS - Performance Results

## Compute Resource

- Distributed-Memory Cluster
- 8 Nodes – 32 Cores
- 2.5 TB of distributed HDFS storage
- On demand



# XPCS - FastCCD2

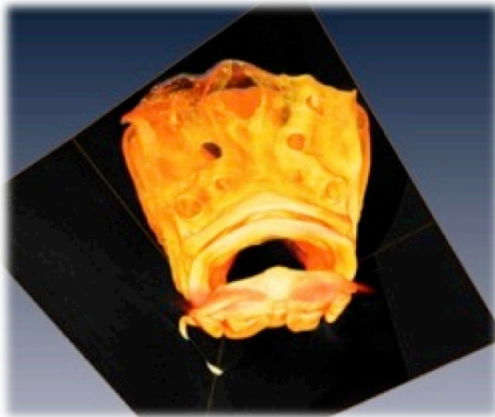
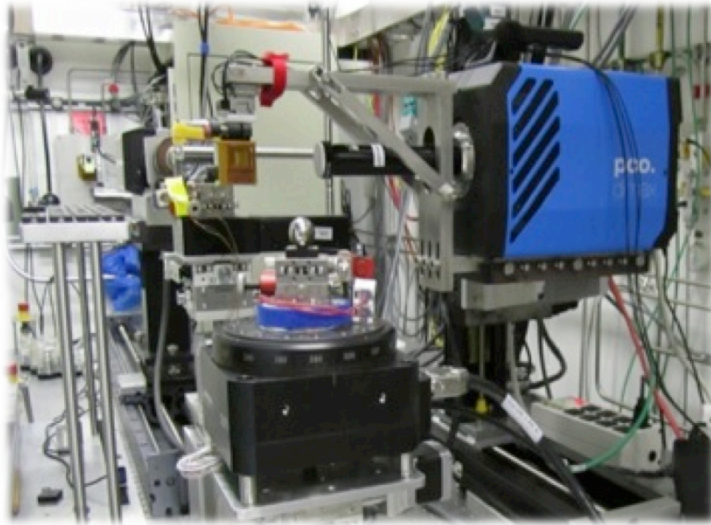


- Custom detector designed by LBNL
- 1K x 1K @ 200 FPS
- Planned to be used by ALS, LCLS, NSLS-II and APS
- ATCA processing crate
- Real-time autocorrelation implementation



# Fast Micro-Tomography

Francesco De Carlo (APS)



Keith Chang (Penn State College of Medicine)

## Beamline and Detector

- 2-BM
- pco.dimax (36GB of onboard RAM)
- 2K X 2K @ 16-bits

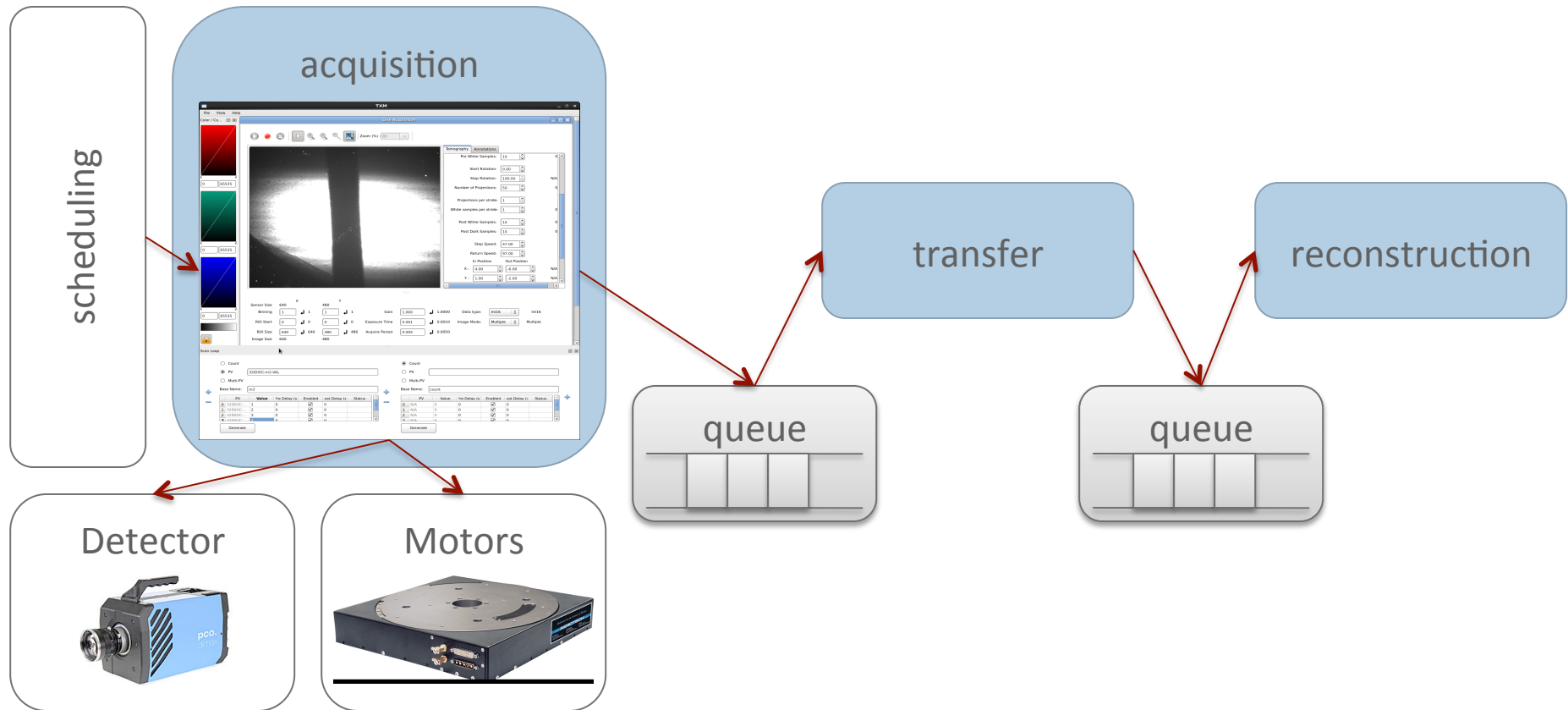
## Tomography Dataset

- Projections around 180 degrees
- ~1,500 FPS
- A few seconds of data collection
- ~1 minute readout
- Up to 11GB raw data per minute

## Reconstruction

- Takes ~5 minutes
- Reconstructed data ~22GB

# Fast Micro-Tomography - Data Workflow





# Multimodal ptychographic nanotomography of roll-coated polymer solar cells

## Beamline and Detectors

- 2-ID-B, 2.5 keV photons, 150 nm focus
- Small-angle: Cornell MMPAD (266×396×150  $\mu\text{m}$  pixels @ 1 ms/frame)
- Fluorescence: SII Vortex-EX SDD (2048 channels/point)

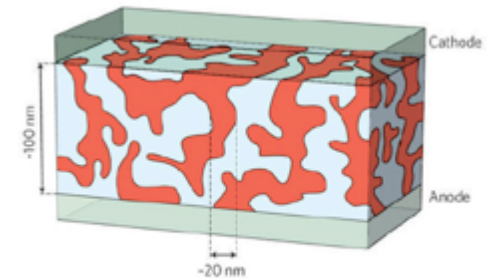
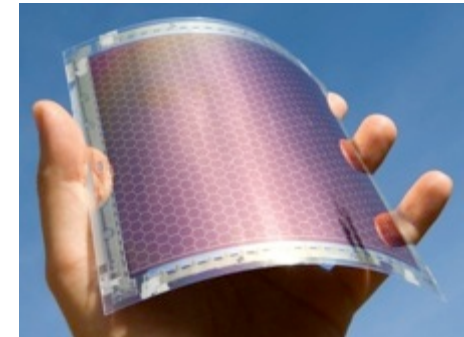
## Tomographic/Ptychographic Dataset

- 70 nm steps, 6 nm pixels (9  $\mu\text{m}$  x 4  $\mu\text{m}$  field)
- 60 projections, recorded every 6°
- 0.1 ms/point, 18 min/projection, 21 h/tomogram
- 129×58 point scan, 7482 diffraction patterns/projection
- **449K diffraction patterns, 176 GB raw data**

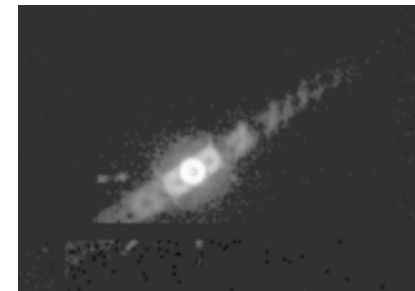
## Reconstruction

- 50 iterations @ 10 min/iteration
- 12 days/reconstruction (24 cores)
- $\Rightarrow$  **308 single-processor compute days!**

D. Vine (APS), J. Andreasen, A. Böttlinger (Risø), K. Green, M. Tate, H. Philipp, S. Gruner (Cornell)

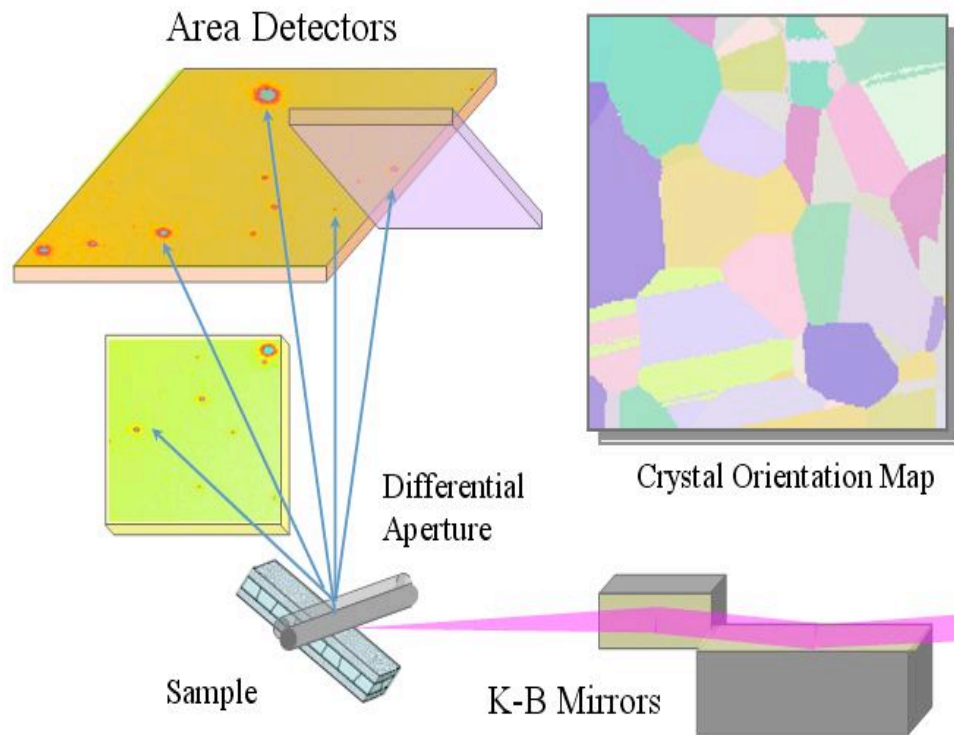


Li *et al.*, Nat. Photon., **6** 153 (2012)



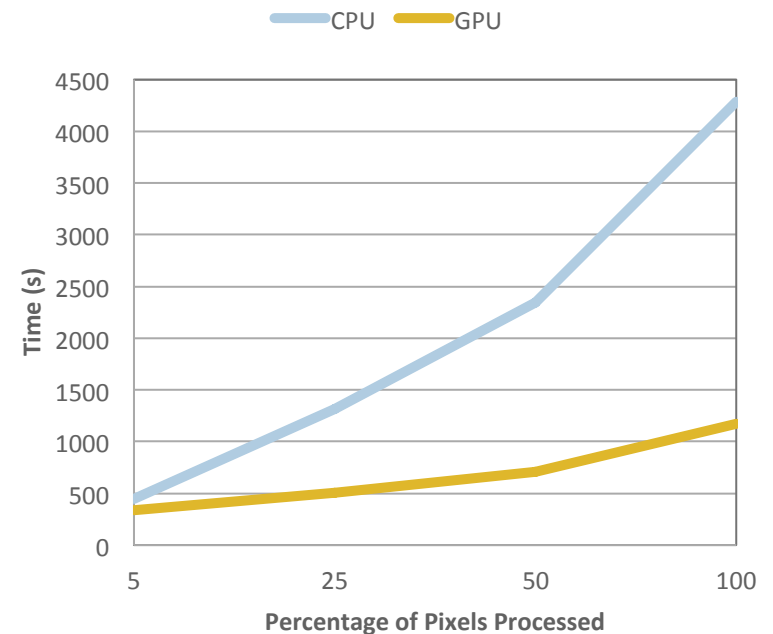
# X-ray Laue Diffraction Microscopy

Jon Tischler (APS)



## GPU Reconstruction

- Large rewrite / refactor of CPU code / algorithm
- Uses Tesla GPU – 6 GB RAM
- ~10 GB of raw data



# User Access to Data





# Globus Online

- Provides access to APS data from the outside
- Used by many user facilities and supercomputing centers
- Optimized bandwidth utilization for faster transfers
- [www.globusonline.org](http://www.globusonline.org)



# Globus Online

The image displays two screenshots of the Globus Online web interface. The top screenshot shows the 'Transfer Files' page with an 'Activate Endpoint: aps#clutch' dialog box overlaid. The dialog box prompts the user to enter credentials for the proxy server 'clutch.aps.anl.gov:51000', including fields for Username, Password, Server DN, and Credential Lifetime. The bottom screenshot shows the same 'Transfer Files' page, but with a file list for the 'aps#clutch' endpoint. The file list includes folders for years 2010-2012, folders like 'springer', 'test', and 'Frazier\_Sam26\_raw', and a file named 'Florian\_2010\_04\_log.txt' with a size of 1MB.

**Top Screenshot: Transfer Files Page**

- Endpoint: rajk#desktop
- Path: /~/
- Endpoint: aps#clutch
- Path: /~/
- Dialog Box: Activate Endpoint: aps#clutch
- Dialog Box Fields: \*MyProxy Server (clutch.aps.anl.gov:51000), \*Username, \*Passphrase, Server DN, Credential Lifetime (hours)
- Buttons: Authenticate, Cancel

**Bottom Screenshot: Transfer Files Page**

- Endpoint: rajk#desktop
- Path: /~/
- Endpoint: aps#clutch
- Path: /data/tomo2/tomo/
- File List:

Item	Type
1a	Folder
529	Folder
ACM	Folder
ACM_Senior_Member	Folder
ALCF_OTP_Myproxy	Folder
BIRN	Folder
Bill_globus_files	Folder
Bill_tutorials	Folder
Biography_short	Folder
CCGrid11_Tutorial	Folder
CDIGS	Folder
CEDPS	Folder
CTS2010	Folder
CV	Folder
C_Programs	Folder
Charts	Folder
Coupons	Folder
CreditReport	Folder
DOE-ASCR-BES-Workshop-2011	Folder
DOE_Terabits_Workshop_Feb2011	Folder
2010_03	Folder
2010_04	Folder
2010_08	Folder
2010_09	Folder
2010_10	Folder
2010_12	Folder
2011_02	Folder
2011_04	Folder
2011_06	Folder
2011_10	Folder
2011_11	Folder
2011_12	Folder
2012_02	Folder
2012_03	Folder
Frazier_Sam26_raw	Folder
beamline_settings	Folder
fzk	Folder
springer	Folder
test	Folder
Florian_2010_04_log.txt	1MB



# Globus Online Catalog

The screenshot displays the Globus Online Catalog interface. At the top, there is a navigation bar with the Globus logo and the text "globus online". To the right of the logo are links for "Manage Data", "Groups", "Support", and "faisal". Below this, there are links for "manage datasets", "start transfer", "view transfer activity", "manage endpoints", and "dashboard".

The main interface includes a search bar with a "Search" button and a "?". Below the search bar is a "Create Dataset" button. On the left side, there is a "Catalog" dropdown menu currently set to "AES", and a "Filter by Annotation" option.

The central part of the interface shows a dataset entry for "control\_cds\_ps75\_180C\_Fq2\_003\_0001-20481.hdf" with a date of "2013-07-30". The owner is listed as "faisal" and the label is empty. Below the dataset name are tabs for "Overview", "Tags", "Sharing", and "Select Files". The "Tags" tab is active, showing an "Edit Tags" section with the following metadata fields:

Field Name	Value
specscan_data_number	180
normalization_method	TRANSMITTED
specfile	simon20120627
output_file_local	/data/exchange/file1
output_data	/exchange1
kinetics	DISABLED
flatfield_enabled	DISABLED
file_mode	MULTI
blemish_enabled	ENABLED
compression	ENABLED

Below the metadata editor, another dataset entry is visible: "R056\_G14\_p01\_30C\_PICCD\_Sq1\_0001-0505.hdf" with a date of "2013-07-30", owner "faisal", and an empty label.

- Bridge across multiple Globus Online endpoints
- User builds meaningful metadata catalogs
- Not a facility-centric perspective of data

# Globus Online Catalog

- Pilot techniques at the APS
- Push data to user specified catalog at end of acquisition
- Read data to a catalog when selected

The screenshot displays the Globus Online Catalog interface. At the top, the header includes the Globus logo and the text 'globus online', along with navigation links for 'Manage Data', 'Groups', 'Support', and the user 'faisal'. Below the header, there are links for 'manage datasets', 'start transfer', 'view transfer activity', 'manage endpoints', and 'dashboard'. On the left side, there is a 'Catalog' dropdown menu currently set to 'AES', a 'Create Dataset' button, and a 'Filter by Annotation' option. The main area shows a search bar with a 'Search' button and a '?' icon. Below the search bar, a dataset entry is visible: 'control\_cds\_ps75\_180C\_Fq2\_003\_0001-20481.hdf' with a date of '2013-07-30', a star icon, and an owner of 'faisal'. An 'Edit Tags' modal is open over this dataset, showing a list of tags with their values and edit icons (pencil icons). The tags and their values are: 'specscan\_data\_number' (180), 'normalization\_method' (TRANSMITTED), 'specfile' (simon20120627), 'output\_file\_local' (/data/exchange/file1), 'output\_data' (exchange1), 'kinetics' (DISABLED), 'flatfield\_enabled' (DISABLED), 'file\_mode' (MULTI), 'blemish\_enabled' (ENABLED), and 'compression' (ENABLED). Below the modal, another dataset entry is partially visible: 'R056\_G14\_p01\_30C\_PICCD\_Sq1\_0001-0505.hdf' with a date of '2013-07-30', a star icon, and an owner of 'faisal'.

# Challenges / Opportunities

- More technique based collaborations
- Tight-knit teams of scientists and software engineers
- Facility integration
- Sustainability – how to keep it working 5 or 10 years in the future?



**Thank you!**