5-WAY MEETING | DATA SESSION

APS DATA POLICY & RESOURCES

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RETENTION POLICY AND PRACTICES

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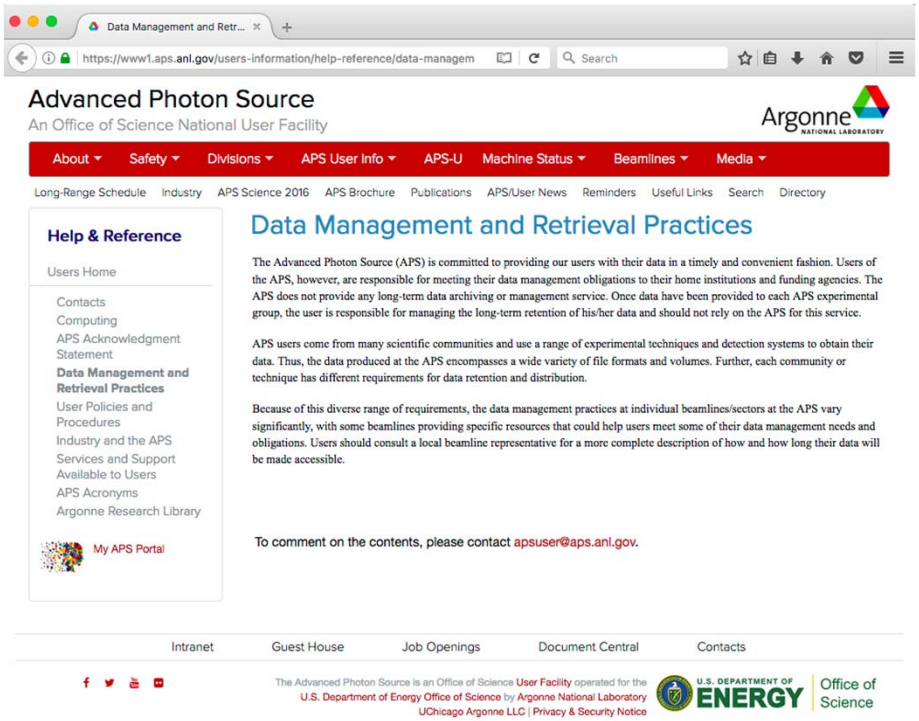
DATA MANAGEMENT & RETRIEVAL

Policy

- The Advanced Photon Source (APS) is committed to providing our users with their data in a timely and convenient fashion.
- Users of the APS, however, are responsible for meeting their data management obligations to their home institutions and funding agencies.
- The APS does not provide any long-term data archiving or management service.
- …user is responsible for managing the long-term retention of his/her data and should not rely on the APS for this service.
- APS will try to keep data for 3 months



https://www1.aps.anl.gov/users-information/help-reference/data-management-retrieval-practices

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DATA MANAGEMENT & RETRIEVAL

Practices

- Retention practices vary; each beamline/technique has its own policy

- Beamlines that have traditionally generated modest amounts of data:
  - Saved much raw data using ‘ad hoc’ storage schemes
  - E.g. floppy disks, external hard drives, local storage arrays, etc.
  - XRF, XPCS, USAXS, and many others

- Metadata is often not stored along with raw data

- Beamlines that are large data producers:
  - Purge data when storage space becomes scarce

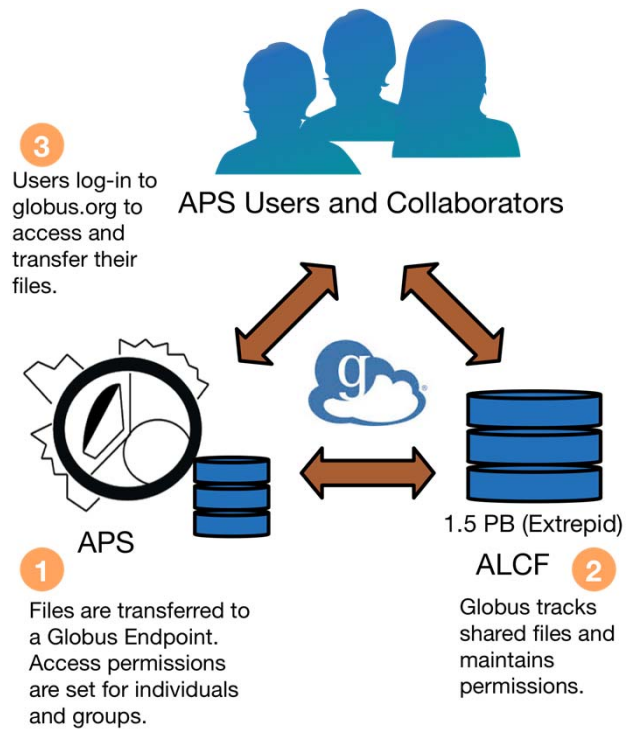
- The APS has made recent strides in this area…

DATA MANAGEMENT & DISTRIBUTION

APS is leveraging storage hardware from the ALCF and software from Globus Services for data management & distribution

- ALCF provides a ~1.5 PB storage system (in building 369) for APS data; ~ 560 TB stored since 2017-1 run
- In use at XSD beamlines and piloted by CATs
- Workflow automation of data and metadata management, access permissions
- *Next: Exploring long-term storage options at ALCF and NERSC | MDF, DOE Data Explorer*

Station	Usage as of 10/2/17	Station	Usage as of 10/2/17
1-ID	440 TB	11-ID-B	542 GB
3-ID	217 MB	11-ID-C	53 GB
DND-CAT	723 GB	CARS	21.1 TB
6-BM (EDD)	301 GB	Bio-CAT	Going Online
6-ID	12 GB	33 (XRIM)	1.4 TB
7-BM	241 MB	34 (XMD)	73 TB
7-ID (FSD)	6.4 TB	DCS-CAT	5 GB
8-ID	17 TB		



Contact: Sinisa Veseli, Roger Sersted Collin Schmitz (APS), William Allcock, Rachana Ananthakrishnan, Ian Foster, Michael Papka (CELS), et al.

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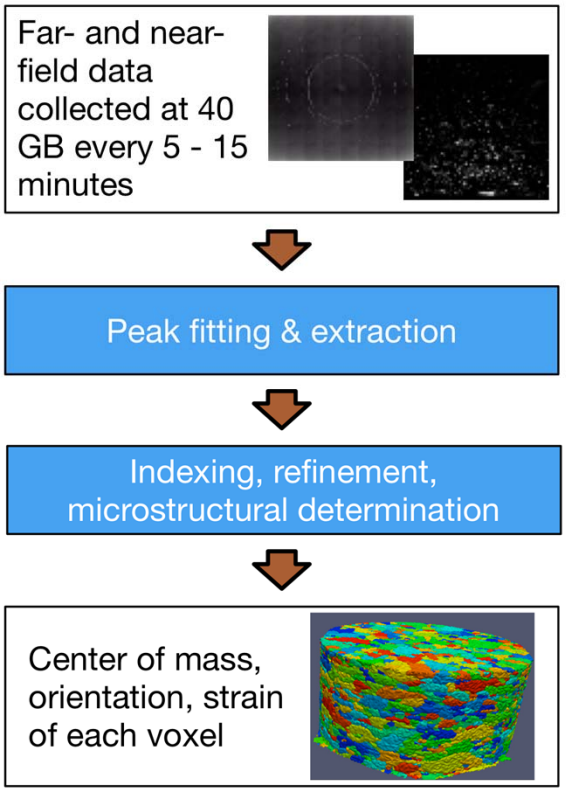
EXTERNAL RESOURCES

HIGH-ENERGY DIFFRACTION MICROSCOPY

NERSC computing resources enable near real-time High-Energy Diffraction Microscopy (HEDM) reconstructions

- Microstructural Imaging with Diffraction Analysis Software (MIDAS) package for HEDM data.
- *160,000 core hour discretionary allocation at NERSC (originally 100,000 core hours); working on ALCC NERSC proposal*
- *Typical turnaround time of ~ 6 minutes using 300 cores on NERSC's real-time queue.*
- *Datasets are small enough that bandwidth to/from NERSC is not an issue.*
- *Requires beamline staff to operate. A data portal is needed for routine use by users.*



Before / After

1K grains / 10K grains

1 core / 300 cores

16 h / 1 minute

25 days / 5 minutes

Total speed-up: ~26 days to ~ 6 minutes with 10x more grains

Contact: Hemant Sharma, Jon Almer
Collaborators: ANL/MCS, ANL/NE, Carnegie Mellon Univ., GE, AFRL, LANL, Cornell, Univ. Tenn., Purdue, et al.

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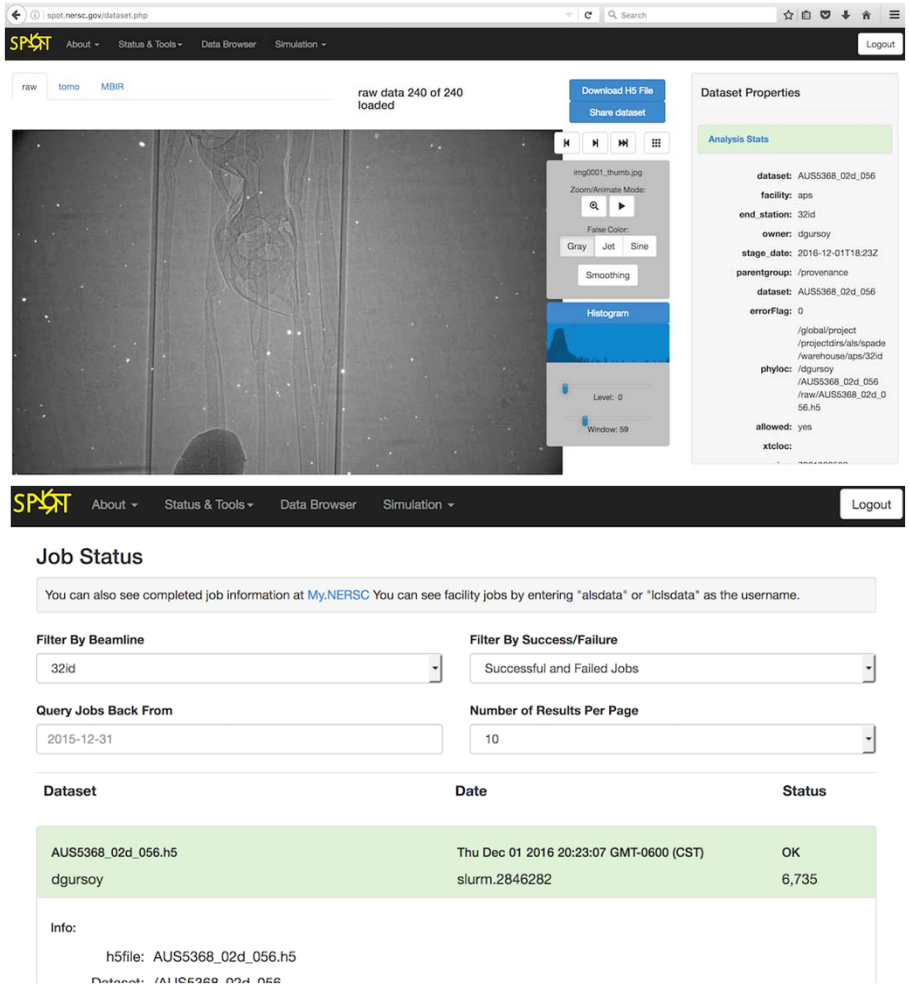
TOMOGRAPHY

SPOT Suite / NERSC Integration Efforts



- Worked with LBNL to integrate APS tomography beamlines with SPOT suite and NERSC for beam time reconstructions
- Achieved rudimentary integration for a demo

- *Overall turn-around time on NERSC is many times slower than when using local compute resources*
- *Systems integration with SPOT suite is incomplete*

Contact: Francesco De Carlo, Doga Gursoy, Brian Toby (APS), Craig Tull, Simon Patton (LBNL), et al.

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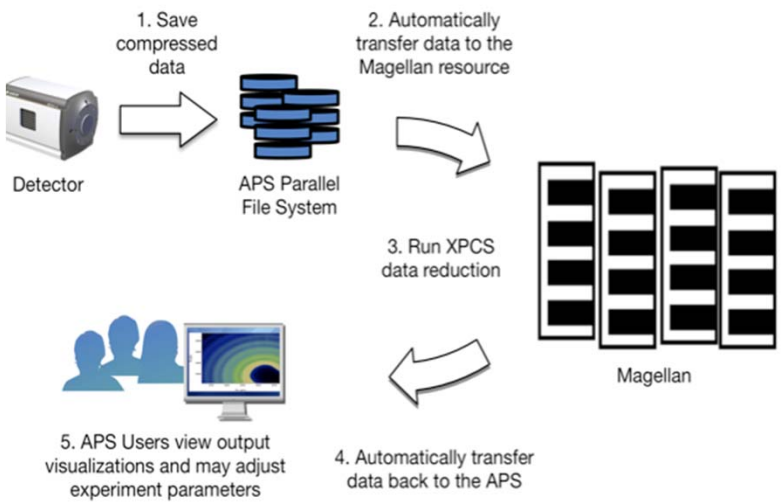
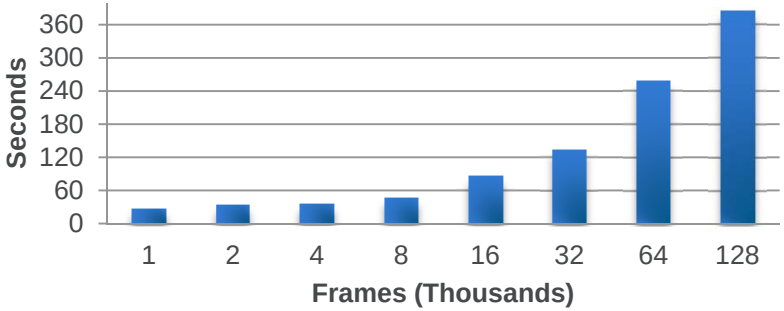
X-RAY PHOTON CORRELATION SPECTROSCOPY (XPCS) ANALYSIS

APS using Argonne's virtualized computing resource for near real-time data reduction



Top: XPCS integrated workflow pipeline depicting data flow from acquisition at APS 8-ID, to Building 240 for computation, and then back to the APS for visualization and interpretation. Bottom: Data reduction performance in seconds for datasets of increasing size measured in number of frames using ten nodes on Magellan.



Magellan

- Argonne's virtualized cloud-computing environment
- Approximately 1,000 node resource
- Located in Building 240
- Connected to the APS via 4 x 10 Gbps links (scalable)

XPCS at APS 8-ID beamline

- XPCS multi-tau Hadoop system set up and running on Magellan
- Fully integrated into the SA-XPCS and WA-XPCS workflow pipelines at 8-ID
- Produces multi-tau and two-time auto-correlation results in near real-time (minutes after data acquisition ends); critical for feedback to conduct experiments

  github.com/AdvancedPhotonSource/xpcs-hadoop

Contact: Faisal Khan, Suresh Narayanan, Alec Sandy, Collin Schmitz, Benjamin Pausma, Nicholas Schwarz (APS), Ryan Aydelott, and Daniel Murphy-Olson (CELS).

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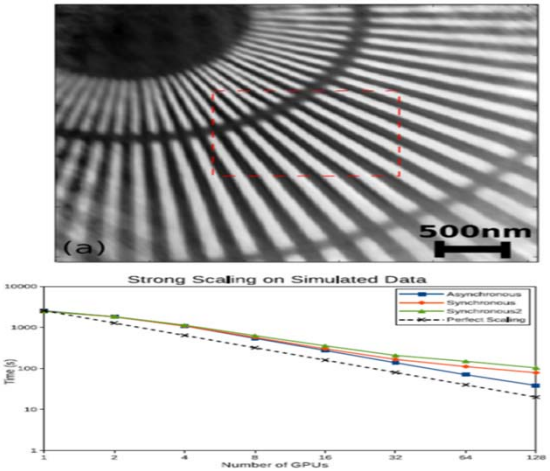
ALCF RELATED R&D PROJECTS

APS leverages ALCF computing resources for software R&D prototypes

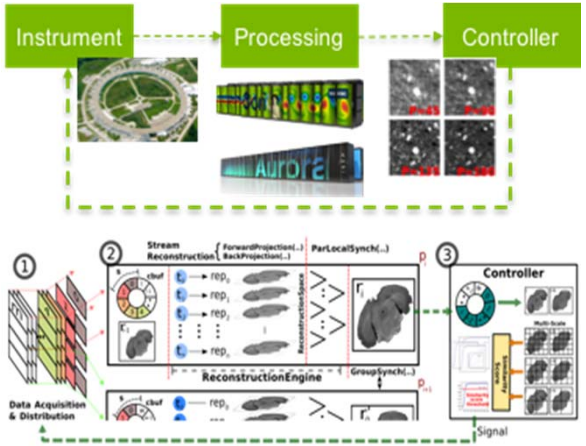


- Software for nanobeam ptychography using leadership scale computing resources
- Reduces real-time image reconstruction by a factor of 52 compared to acquisition time
- Runs on to 128 GPUs at the ALCF

Y Nashed, C Jacobsen, D Vine, J Deng, R Harder, E Vacek, K Yue, D Ming, et al.

- New high-performance code for x-ray fluorescence elemental mapping
- High-performance data processing opens the potential to analyze data in near real-time as it streams from the detector
- Successful tests on ALCF's Theta

A Glowacki, Z (Wendy) Di, S Vogt, et al.



- MONA: Smart system that couples acquisition, analysis, and feedback for adaptive experiment control
- Prototype: Streamed materials data from TXM to ALCF for iterative reconstruction; stopped acquisition when data quality was sufficient

D Gursoy, T Bicer, V De Andrade, X Yang, R Kettimuthu, I Foster, F De Carlo, et al.

FUTURE NEEDS / WORKING TOGETHER

- In order to operate a facility and cope with anticipated increases in data (both pre- and post- APS-U), anticipate need for a multiple order-of-magnitude increase in storage capacity coupled with compute resources.
- The capability of individual user groups to cope with data will not scale.
- Push from user community to manage the full data life-cycle and provide the easy ability to share, search, and mine data after experiment time.

1. Can we work toward centralized funding/support for using NERSC storage for long-term archival? Same for ESnet?
2. Clarification/agreement of role of facilities.
3. In order to maximize use off-site computing and storage resources (e.g. NERSC) the light sources should take ownership of systems integration, optimization, data portals, etc. (like other scientific domains).
   - Recommend a working group to develop a plan and estimate.

THANK YOU FOR YOUR TIME