5-WAY MEETING

# THE 5 BES LIGHT SOURCE DIRECTORS' DATA WORKING GROUP – STATUS UPDATE

April 23, 2018
Advanced Light Source

# MEMBERS

**Stuart Campbell**

Group Leader, Data Acquisition, Management, and Analysis

National Synchrotron Light Source II (NSLS-II)

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Research Scientist, Experimental Systems Group

Advanced Light Source (ALS)

**Amedeo Perazzo**

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Linac Coherent Light Source (LCLS)

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Group Leader, Scientific Software Engineering & Data Management

Advanced Photon Source (APS)

# PURPOSE

- The Data Working Group (DWG) was formed after the 5-Way meeting in October 2017.
- The Facility Directors recognize the importance of working together in the data and computing space.
- Serve as a resource for the 5 BES Light Source Facility Directors to provide information and recommendations on working together in the areas of data and computing.

Two tasks:

1. Report on Data Retention – Completed: March 21, 2018
2. Report on Real-time Computing Needs – In Progress

# REPORT ON DATA RETENTION

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# DATA RETENTION CHARGE

## Explore the topic of data retention at the 5 facilities

Outline ways for the light sources to work together collaboratively toward a more uniform long-term approach to data retention

- Current data retention policies and practices
- Recommendations for a common data retention policy template (including an open access policy after an embargo period)
- Present scenarios for implementing possible data retention policies
- Analysis of materials and labor costs (FY18 dollars and FTEs)
- Identify major challenges

# CURRENT STATUS AT THE FACILITIES

Each facility, and in some cases, individual instruments, have their own unique tools and practices with different levels of saturation, levels of maturity, and data retention time frames:

**LCLS** – The only facility that has a complete long-term tape-based storage and retrieval solution in production use; Data on accessible tape for 10 years; Funded by the facility and its host institution

**ALS** – Utilizes NERSC and the prototype SPOT suite for storage at 1 to 3 beamlines; Stored 3 PB so far; No minimum guarantee

**APS** – Modest central storage system, and has begun to roll-out a standard set of tools to beamlines (currently 20 end-stations); Many instruments have local solutions; No minimum guarantee

**NSLS-II** – Data is stored on beamline local systems; commissioning a PB-order storage system for use with its *databroker* tools; Retains data for a minimum of 1 year

**SSRL** – Storage servers divided among three divisions; Retention varies from 1 to 10 years

# SYNOPSIS

## Current state of data management capabilities and deployment saturation at each light source

| Capability | Facility | | | | |
|---|---|---|---|---|---|
| | ALS | APS | LCLS | NSLS-II | SSRL |
| **Archival Storage** | (Prototype) NERSC | None | (Production) LCLS/SLAC/NERSC | None | None |
| **Facility Central Storage** | (Prototype) NERSC | (Production) APS | (Production) LCLS | (Prototype) NSLS-II | (Production) SSRL |
| **Management Tools** | (Prototype) SPADE | (Partial) APS Data Mgt. System | (Production) iRODS | (Partial) NSLS-II databroker | None |
| **Catalog & Database** | (Prototype) SPOT Suite | (Prototype) APS Data Mgt. System | (Production) iRODS, MySQL | (Production) NSLS-II databroker | None |
| **Web Portal** | (Prototype) SPOT Suite | (Prototype) APS Data Mgt. System | (Production) LCLS ELog | None | (Planned) User Portal |
| **Authentication & Authorization** | (Prototype) NERSC Accounts | (Production) APS Accounts | (Production) SLAC Accounts | None | (Production) SSRL Accounts |
| **External Data Lifecycle Tools** | None | None | None | None | None |
| **Instruments Deployed** | 1 - 3 | 20 | ALL | ALL | ALL |

# ARCHIVAL STORAGE COST COMPARISON

## DOE storage facilities are currently more cost effective than commercial cloud vendors for today's light source needs

| NERSC Tape Archive | PB | Duration (Years) | | | |
|---|---|---|---|---|---|
| | | 1 | 3 | 5 | 10 |
| HPSS System at NERSC | 0.5 | $5,200 | $15,600 | $26,000 | $52,000 |
| | 1 | $10,400 | $31,200 | $52,000 | $104,000 |
| | 2 | $20,800 | $62,400 | $104,000 | $208,000 |
| | 5 | $52,000 | $156,000 | $260,000 | $520,000 |
| | 10 | $104,000 | $312,000 | $520,000 | $1,040,000 |
| **Amazon Tape Archive** | PB | Duration (Years) | | | |
| | | 1 | 3 | 5 | 10 |
| Amazon Glacier tape storage | 0.5 | $12,583 | $37,749 | $62,915 | $125,829 |
| | 1 | $25,166 | $75,498 | $125,829 | $251,658 |
| | 2 | $50,332 | $150,995 | $251,658 | $503,317 |
| | 5 | $125,829 | $377,488 | $629,146 | $1,258,292 |
| | 10 | $251,658 | $754,975 | $1,258,292 | $2,516,584 |
| **FNAL Tape Archive** | PB | Duration (Years) | | | |
| | | 1 | 3 | 5 | 10 |
| SAMGrid tape storage system | 0.5 | $17,920 | $53,760 | $89,600 | $179,200 |
| | 1 | $35,840 | $107,520 | $179,200 | $358,400 |
| | 2 | $71,680 | $215,040 | $358,400 | $716,800 |
| | 5 | $179,200 | $537,600 | $896,000 | $1,792,000 |
| | 10 | $358,400 | $1,075,200 | $1,792,000 | $3,584,000 |
| **NERSC Fast Disk Storage** | PB | Duration (Years) | | | |
| | | 1 | 3 | 5 | 10 |
| Cost of new spinning disk storage at NERSC | 0.5 | $30,000 | $90,000 | $150,000 | $300,000 |
| | 1 | $60,000 | $180,000 | $300,000 | $600,000 |
| | 2 | $120,000 | $360,000 | $600,000 | $1,200,000 |
| | 5 | $300,000 | $900,000 | $1,500,000 | $3,000,000 |
| | 10 | $600,000 | $1,800,000 | $3,000,000 | $6,000,000 |
| **Amazon Fast Disk Storage** | PB | Duration (Years) | | | |
| | | 1 | 3 | 5 | 10 |
| Amazon S3 storage | 0.5 | $150,995 | $452,985 | $754,975 | $1,509,949 |
| | 1 | $301,990 | $905,970 | $1,509,949 | $3,019,899 |
| | 2 | $603,980 | $1,811,939 | $3,019,899 | $6,039,798 |
| | 5 | $1,509,949 | $4,529,848 | $7,549,747 | $15,099,494 |
| | 10 | $3,019,899 | $9,059,696 | $15,099,494 | $30,198,988 |

| Amazon Egress Charges | PB | Duration (Years) | | | |
|---|---|---|---|---|---|
| | | 1 | 3 | 5 | 10 |
| Additional cost to move data from Amazon resources; charge is $740,000 to move 1 PB in one year | 0.5 | $370,000 | $1,110,000 | $1,850,000 | $3,700,000 |
| | 1 | $740,000 | $2,220,000 | $3,700,000 | $7,400,000 |
| | 2 | $1,480,000 | $4,440,000 | $7,400,000 | $14,800,000 |
| | 5 | $3,700,000 | $11,100,000 | $18,500,000 | $37,000,000 |
| | 10 | $7,400,000 | $22,200,000 | $37,000,000 | $74,000,000 |
| **Google Coldline Storage** | PB | Duration (Years) | | | |
| | | 1 | 3 | 5 | 10 |
| Infrequently accessed data storage; data must be stored for at least 90 days to avoid additional costs | 0.5 | $44,040 | $132,121 | $220,201 | $440,402 |
| | 1 | $88,080 | $264,241 | $440,402 | $880,804 |
| | 2 | $176,161 | $528,482 | $880,804 | $1,761,608 |
| | 5 | $440,402 | $1,321,206 | $2,202,010 | $4,404,019 |
| | 10 | $880,804 | $2,642,411 | $4,404,019 | $8,808,038 |
| **Google Nearline Storage** | PB | Duration (Years) | | | |
| | | 1 | 3 | 5 | 10 |
| Infrequently accessed data storage; data must be stored for at least 30 days to avoid additional costs | 0.5 | $62,915 | $188,744 | $314,573 | $629,146 |
| | 1 | $125,829 | $377,487 | $629,146 | $1,258,291 |
| | 2 | $251,658 | $754,975 | $1,258,291 | $2,516,582 |
| | 5 | $629,146 | $1,887,437 | $3,145,728 | $6,291,456 |
| | 10 | $1,258,291 | $3,774,874 | $6,291,456 | $12,582,912 |
| **Google US Multi-Regional Storage** | PB | Duration (Years) | | | |
| | | 1 | 3 | 5 | 10 |
| Fast storage for routine access; egress charges apply | 0.5 | $163,578 | $490,734 | $817,889 | $1,635,779 |
| | 1 | $327,156 | $981,467 | $1,635,779 | $3,271,557 |
| | 2 | $654,311 | $1,962,934 | $3,271,557 | $6,543,114 |
| | 5 | $1,635,779 | $4,907,336 | $8,178,893 | $16,357,786 |
| | 10 | $3,271,557 | $9,814,671 | $16,357,786 | $32,715,571 |

# STRATEGY AND RECOMMENDATIONS

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# STRATEGY

## Moving forward together

- Each facility should continue to expand its data management capabilities
- Develop and share back-end tools needed to integrate with the interfaces provided by archival data storage providers
- As capabilities develop, the facilities can then together look at common developments in user data portals and metadata catalogs
- Fill-in the missing gaps in features across the facilities, especially where little effort has been devoted
  - value-added data lifecycle tools
  - common user authentication and authorization mechanisms
- Adopt a common template for data retention
- Engage with ASCR and others towards developing state-of-the-art data management systems and tools

# CAPABILITIES NEEDED TO ACHIEVE LONG-TERM DATA RETENTION

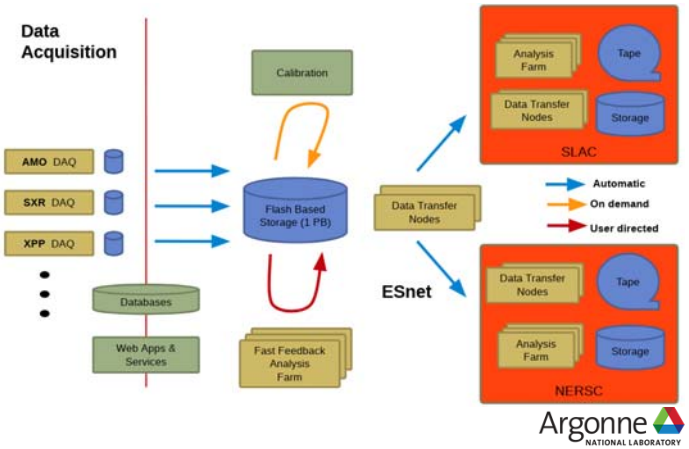
Achieving long-term data retention and full data lifecycle management of light source data requires the implementation of a number of high-level capabilities.

**Facility Storage**

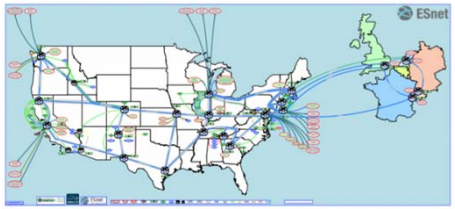
- Short-term, high-reliability, very fast data buffer – part of data acquisition scheme
- Sized for each facility's needs: one or two facility run cycles (6 – 12 months)
- Forms: a central system (most cost effective), or distributed systems that share similar architecture and software stack

**Archival Storage**

- Storage for 10+ years
- Today, tape is the most economical; object-storage systems may be so in the future
- Simple cost analysis of NERSC, FNAL, Amazon, and Google



# CAPABILITIES NEEDED TO ACHIEVE LONG-TERM DATA RETENTION




**Networking (across the light source facilities, the HPC facilities, and the users' institutions)**

- ESnet's 100 Gbps backbone, 8.8 Terabit network should suffice for piloting utilizing wide-area resources for long-term archival
- Network bandwidth will need to be expanded by one order of magnitude in the coming years (the ESnet6 upgrade will reach 1 Tbps by 2022)

**Software Tools**

- *Storage Management Tools:* Data transfer and permission management, e.g. Globus, HPSS tape system integration, ACLs, iRODS, Rucio
- *Catalogs & Databases:* Searchable data and metadata
- *Portal:* Web and mobile portals for easy access
- *Authentication & Authorization:* Desired SSO or federated IDs (ORCiD, Globus, umbrellaID)
- *External Lifecycle Tools:* DOI minting (OSTI), domain specific databases

ESnet Energy Sciences Network

iRODS CONSORTIUM

globus online

Shibboleth

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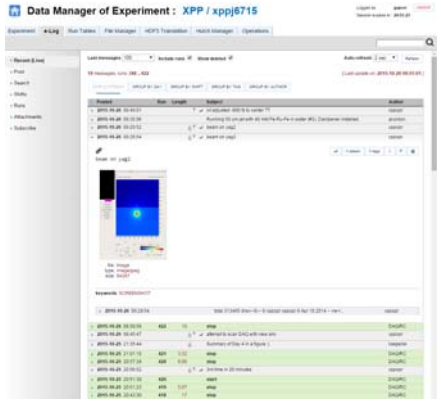
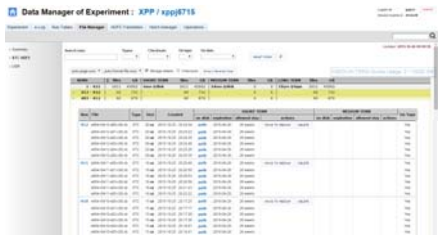
# NEXT STEPS

## Must have capabilities

- *Policy* – Each facility adopt a uniform policy template
- *Facility Storage* – If not already existing, each facility should develop and implement an internal storage strategy - dedicate between 0.25–0.5 FTE per year
- *Archival Storage* – Begin a pilot project with one storage provider (onsite or offsite)
- *Management Tools* – Together the facilities with internal development effort can work on developing shared tools for interfacing with either the HPSS, AWS, or SAMgrid archival interface systems, requiring 1–2 FTE of combined effort
- *Catalog & Database* – Facilities should together evaluate the existing solutions on a technical level, and generate an action plan moving forward - this exploratory work is estimated to require about 1 FTE of combined effort
- *Web Portal* – Facilities should together evaluate the existing solutions on a technical level, and generate an action plan moving forward - this exploratory work is estimated to require about 1 FTE of combined effort



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# NEXT STEPS

## Nice to have

- *Authentication & Authorization* – Organize a working group to evaluate potential options and recommend a path forward (some R&D aspects)
- *External Data Lifecycle Tools* – Collaboratively investigate the use of external data lifecycle management tools, including the DOE Digital Object Identifier minting service, the DOE Data Explorer, and other external tools - a common set of tools can be developed and used by each facility, requiring 2–3 FTE of combined effort
- *Open Access* - Develop a strategy for soliciting user engagement (possibly at Users Meetings and User Executive Committee), and perform a cost-benefit analysis for an open access data policy
- *In addition to the above investigation and development effort, each facility should plan to resource, at a minimum, approximately 1 FTE per year for successful deployment, integration, and maintenance related tasks*

# A COMMON DATA RETENTION POLICY TEMPLATE

# POLICY TEMPLATE

## Recommend adoption of a common policy template

There is often a difference between stated data policies and actual data practices. In many cases actual practices exceed the stated policies. The policy is not often a useful guide as to what one should expect!

***Recommendation:*** The Data Working Group recommends that each facility adopt a uniform high-level policy template, with an optional second level:

- The high-level policy allows each facility to indicate the expected time frames over which data may be retained, aligned to each facility's needs, resources, and constraints
- It can also inform users as to their responsibilities regarding data management, and statements concerning data ownership and embargo periods
- The second level can be used by facilities with heterogeneous data management environments

# POLICY TEMPLATE

Draft Data Retention Policy Template

The user community and its sponsoring organizations are very diverse with differing requirements for data retention. The <Facility Name> cannot guarantee indefinite data archival.

Users of the <Facility Name> are responsible for meeting the data management requirements of their home institutions and funding agencies. Once data have been provided to the user group, the user group is responsible for managing the long-term retention of their data.

[The user group will have sole access to the data during a <Duration> embargo period, renewable if necessary. After the embargo, the data may be released for open access.]

The ownership of data generated at the <Facility Name> is governed by the User Agreement in place between the user's institution and the contractor that operates the facility. Refer to your User Agreement for more details.

Draft Data Retention Practices Template

The <Facility Name> is committed to providing its users with their data in a timely and convenient fashion. Experiment data and metadata collected at the <Facility Name> may be stored at and retrieved from the facility <for up to | for at least Duration>. [Analyzed data may be stored at and retrieved from the facility <for up to | for at least Duration>.] [Please refer to instrument specific supplemental data policies for more details.]

Draft Supplemental Data Retention Information
(Instrument Specific)

- Instrument or beamline name
- Types (raw and analyzed) and sources of data and metadata
- Content and format of data and metadata
- Duration of data and metadata preservation
- Access mechanism information

# DISCUSSION ITEMS

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# OPEN DATA ACCESS

**Pros:**

- In some fields, data re-use has led to significant numbers of publications beyond those first generated by the original experimentalists
- Access to previously collected data may help users better plan and use their beam time
- The adoption of an open data access policy may help increase the scientific impact of the facilities
- This will create an entirely new class of facility users: *light source data users*.
- Technically feasible to accomplish

**Concerns:**

- While welcome by many users, this may be opposed by other users
- Requires effort to collect sufficient experiment and sample metadata

***Recommendations:*** Develop a strategy for soliciting user engagement, and perform a cost-benefit analysis

# ANALYZE REAL-TIME COMPUTING USE CASES FOR A NUMBER OF REPRESENTATIVE TECHNIQUES

These techniques will be chosen to form a representative cross-cut of techniques requiring capabilities that are currently or soon will be pushing the boundaries of real-time computing needs, and are aligned with planned instrument and facility upgrades.

Initial focus areas:

- GISAXS
- Micro-Diffraction for materials studies
- Ptychography
- Spectroscopy
- Tomography
- XPCS
- Nanocrystallography
- Single Particle Imaging

# THANKS FOR YOUR TIME

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