

# Managing Experiment Data with Ease at the Advanced Photon Source



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# Advanced Photon Source (APS)

## Argonne National Laboratory

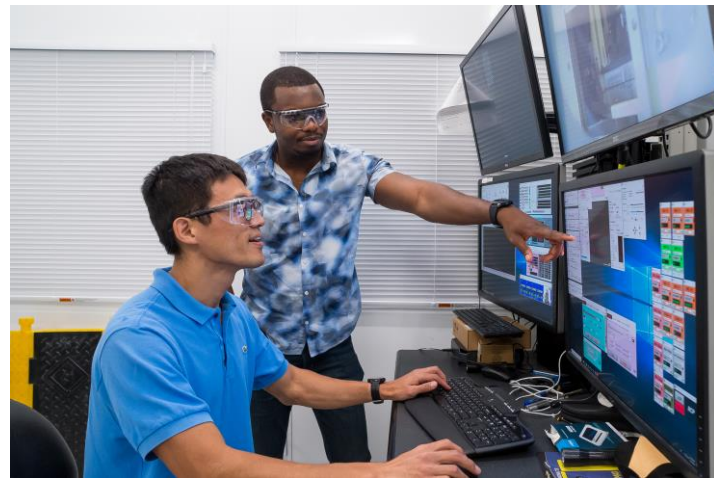
- Wavelengths of the emitted photons span a range of dimensions from the atom to biological cells
- Scientific user facilities (5 funded by the US Department of Energy)
- Serves thousands of users per year from academia, government, and industry
- Diverse communities: materials research, biology, geosciences, life sciences, security, and many more



Advanced Photon Source (APS) at  
Argonne National Laboratory

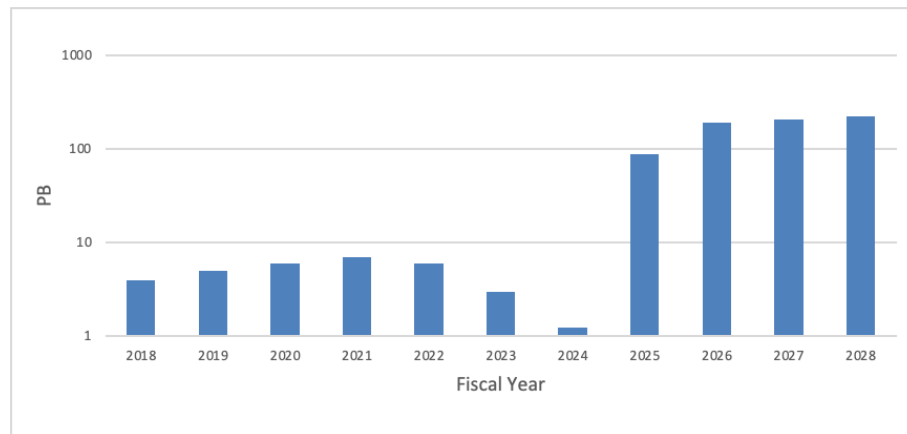
# Data Generation at the APS

- 66 operating beamlines that house over 100 unique instruments
- About 6,000 annual experiments performed by over 5,500 facility users each year
- Approximately 7PB of raw experimental data per year
- The amount of data generated at the APS continues to quickly increase due to advances in new measurement techniques, detectors, instrumentation, and data processing algorithms



# Data Generation at the APS

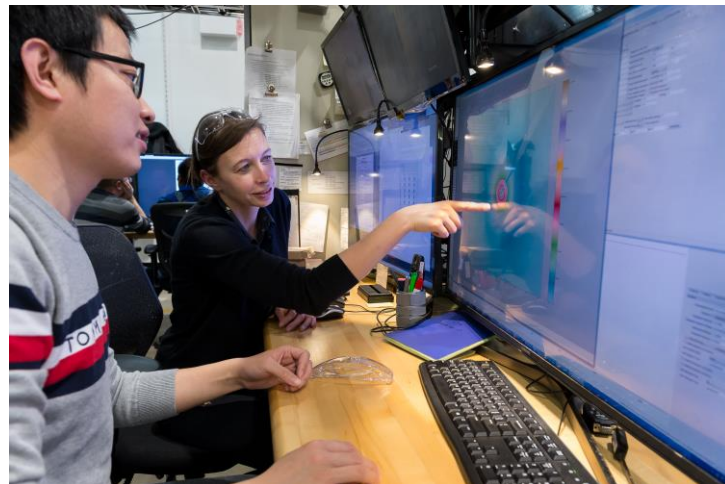
- In April of 2023, the APS will undergo a massive upgrade that will replace the current electron storage ring
- Once the upgraded APS storage ring and beamlines are commissioned and brought into operation, it is estimated that the volume of data generated at the APS will increase by at least two orders of magnitude to 100s of PBs of raw data per year



Estimated data generation volumes per year at the APS. Data generation will drop temporarily due to the installation of storage ring and beamline upgrades.

# Challenges for Data Management

- Beamlines have multiple experiment techniques, types of detectors, data rates, data formats, operating systems, and processing workflows
- Users come from different research institutions, universities, and industries, and must be able to access their data after leaving the facility
- Users access data immediately or several years after it is created. They may be conducting experiments independently and remotely, or in person with close involvement with beamline staff.
- Beamline scientists have different levels of technical expertise.

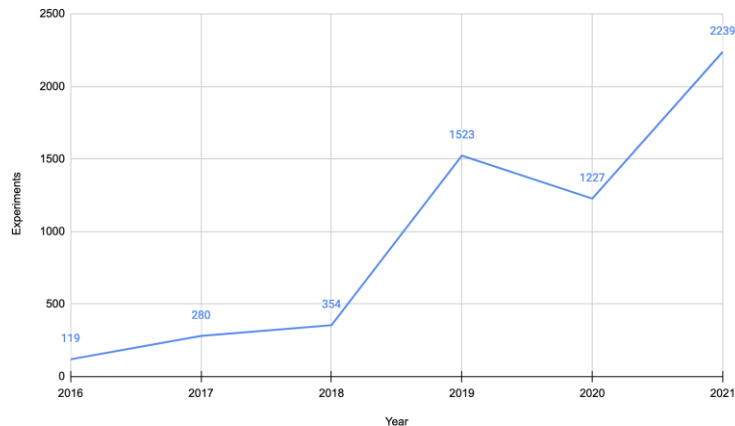
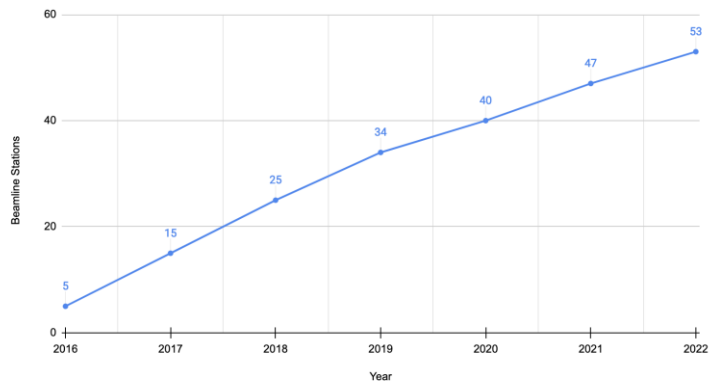


# The Data Management System at the APS

- Specific data management needs typically vary from beamline-to-beamline, mostly depending upon the types of detectors, X-ray techniques, and data processing tools in use
- However, most of the data management requirements are related to a set of tasks common to all beamlines:
  - *Storage area management* (e.g. movement of acquired data from local storage to a more permanent location, data archival, etc.)
  - *Enabling users and applications to easily find and access data* (metadata and replica catalogs, remote data access tools)
  - Facilitating data processing and analysis with automated or user-initiated processing workflows

# Impact of the Data Management System

Adoption of Data Management at the APS



- October 2015: First DM software deployment at 6-ID-D
- December 2016: 5 beamline deployments, about 150 TB used storage
- September 2022: 53 beamline deployments, about 3.3 PB of used storage space, over 7400 experiments in DM DB



# APS Data Management System

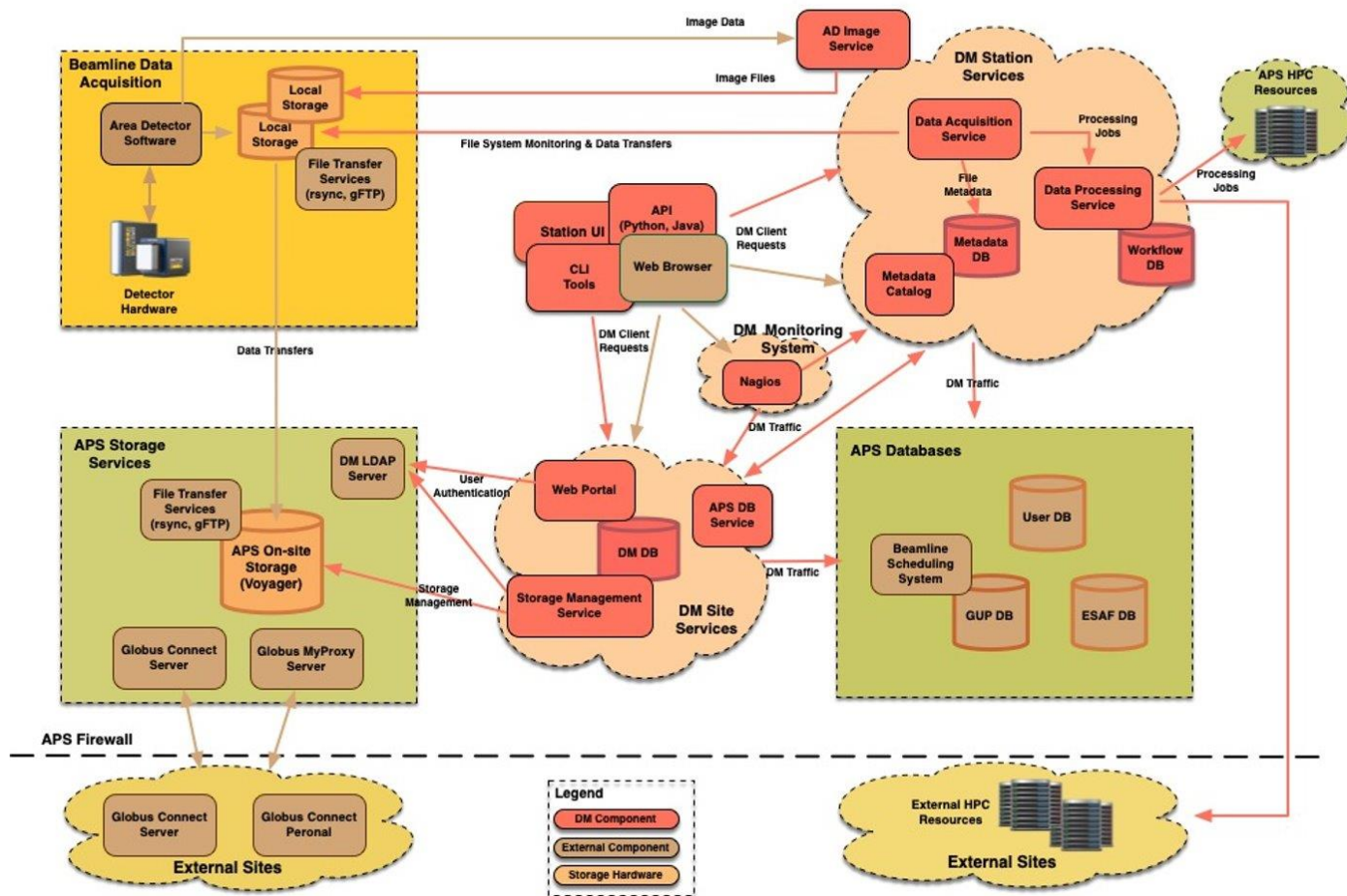
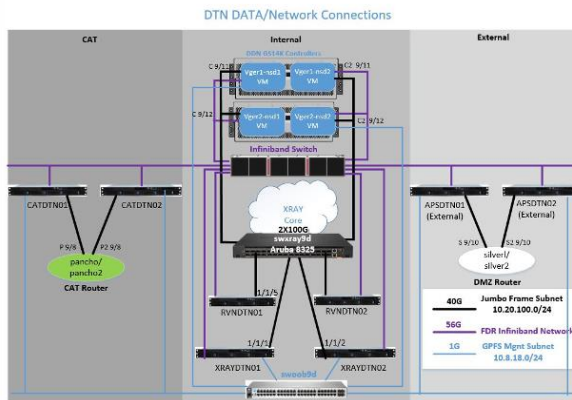
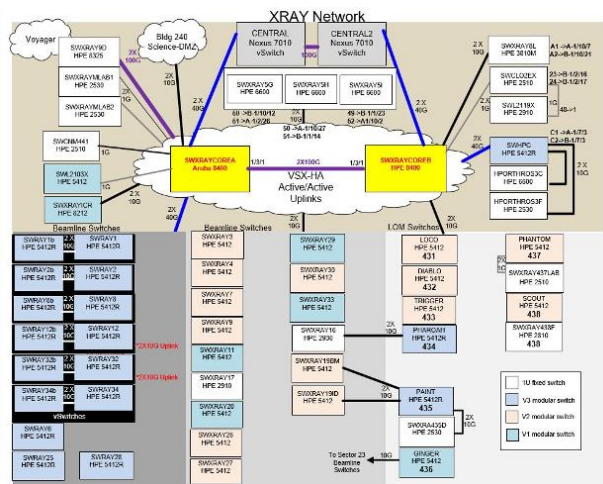




Diagram illustrating the Data Direct Networks GS14KX GridScaler Data Storage Appliance connected to a server rack. The appliance is shown on the left, and the server rack is on the right. The connection is labeled as 4 X 56 Gbps. The server rack contains HPE DL360 Gen10 nodes, with connections for 4 X 40 Gbps to the APS Beamline Network, 2 X 40 Gbps to the ALCF, and 2 X 40 Gbps to the STFT - Public Internet. The total connection for the server rack is 8 X 56 Gbps.



## HPE 3Par Family

# Infrastructure

## Network

- 6 XSD beamline switches have 40G links to core switches
- Most beamline/LOM switches have 10G links to core switches
- Each data transfer node for the central storage system has 40G link

## Storage

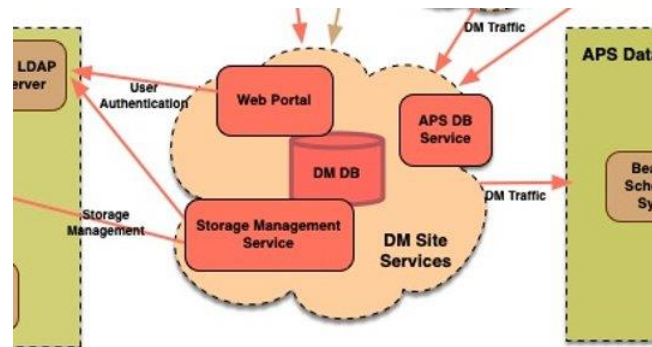
- GridScaler GS14KX file storage appliance, 6PB storage
- 8 Data Transfer Nodes: 1 Intel Xeon 6144 3.5GHz CPU, 128GB RAM, 40 Gbps ethernet link, 56 Gbps Infiniband, 2 x 400GB SSD drives (mirrored)

## Virtualization

- HPE ProLiant Blade System: 2 x c7000 chassis
- 26 hypervisors: HPE ProLiant BL460c blade servers, dual CPU, 36 hyper-threaded cores per CPU, between 128 GB and 512 GB RAM
- Two HPE 3Par storage arrays
- Hypervisor nodes support 8 virtual clusters

# Site Services

- DM Database (PostgreSQL)
  - Maintains information about users, experiments, and beamline deployments
- Storage Management Service (Python, REST)
  - Runs on the storage head node
  - Provides experiment management services
  - Interacts with LDAP and APS Databases
  - Controls storage file system permissions, which enables data access for remote users
- APS DB Service (Python, REST)
  - Enables easy access to ESAF and GUP information
- Automated utilities for synchronizing DM user information with APS User Database



- Every DM service has a set of monitoring interfaces that enable external applications to find out about its state
- These are used by the custom Nagios plugins that provide up-to-date information about the health of the DM station deployments

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# User Interfaces

- DM Station GUI
  - Implemented in PyQt
  - Uses Python REST APIs
- Extensive set of command line tools
  - Built on top of Python APIs
  - Session based
  - Fully scriptable
  - Usage documentation (--help option)
- Python REST services are accessible via API
  - DM Python modules available as Conda packages
  - Easy access to ESAF DB and Beamline Scheduling System

DM Station: HPCAT

Experiments DAQs Uploads Workflows Processing Jobs Settings

Back test-6.1.4-081122-01 Settings View Files File Collection Stats

Name: test-6.1.4-081122-01

Start Date: 4/15/22 End Date: 4/16/22

Type: TEST

Description: sure-induced phase transformation under variable loading rate

Storage Root Path: Storage Root Path

Save

Modify Users

Data Directory or Single File Path: Data Directory or Single File Path Browse

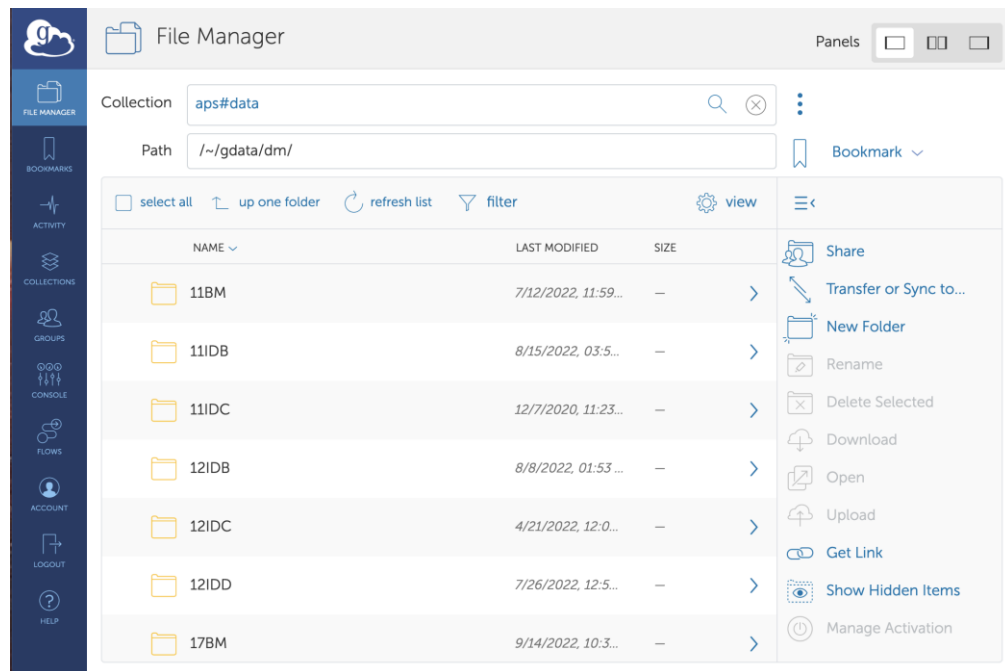
Additional Parameters: Param1:Value1,Param2:Value2, ...

Initialize Start DAQ Start Upload Finalize

	Username	First	Last	Email
1	d313944	Hannah	Parraga	HPARRAG
2	d225159	Sinisa	Veseli	SVESELI@
3	d37309	John	Hammonds	HAMMONI
4	d316508	Steven	Henke	SHENKE@
5	d219224	Nicholas	Schwarz	NSCHWAF

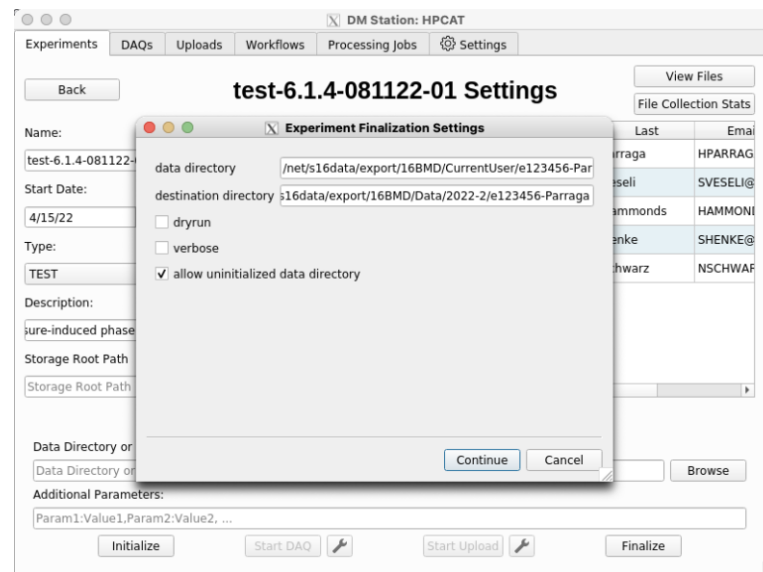
# Data Access

- Globus Endpoint on data storage node provides secure access to users
- Authentication with APS user credentials
- Data access from any location at any time during and after the experiment



# Local File Permissions

- Experiment data directories on local beamline machines can be "initialized" and "finalized"
- File permissions and access control lists can be set so that only the beamline administrator or allowed user group has access to the data local after the experiment is complete.

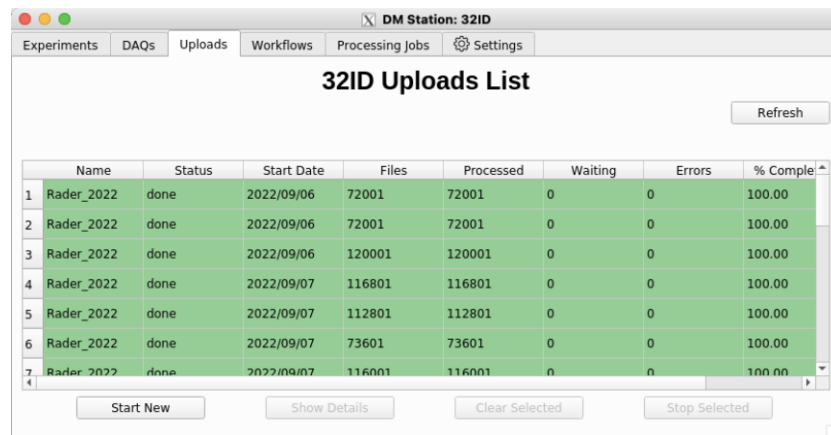




# Station Services: DAQ Service

- Each beamline deployment (“DM Station”) includes several Python services accessible via REST interfaces: DAQ Service, Metadata Catalog and Processing Service

- Data Acquisition Service
  - Responsible for data uploads and for monitoring local file storage
  - Customizable, plugin-based processing framework



The screenshot shows a web application window titled "DM Station: 32ID". It has a navigation bar with tabs: Experiments, DAQs, Uploads, Workflows, Processing Jobs, and Settings. The "Uploads" tab is selected, displaying the "32ID Uploads List". A "Refresh" button is in the top right. Below the title is a table with columns: Name, Status, Start Date, Files, Processed, Waiting, Errors, and % Complete. The table contains 7 rows of data, all with a status of "done". At the bottom of the interface are four buttons: "Start New", "Show Details", "Clear Selected", and "Stop Selected".

	Name	Status	Start Date	Files	Processed	Waiting	Errors	% Complete
1	Rader_2022	done	2022/09/06	72001	72001	0	0	100.00
2	Rader_2022	done	2022/09/06	72001	72001	0	0	100.00
3	Rader_2022	done	2022/09/06	120001	120001	0	0	100.00
4	Rader_2022	done	2022/09/07	116801	116801	0	0	100.00
5	Rader_2022	done	2022/09/07	112801	112801	0	0	100.00
6	Rader_2022	done	2022/09/07	73601	73601	0	0	100.00
7	Rader_2022	done	2022/09/07	116001	116001	0	0	100.00

# Station Services: Metadata Catalog

- Metadata Catalog (MongoDB)
  - Metadata are arbitrary key/value pairs
  - Each experiment has its own file metadata collection
  - File metadata can be retrieved using command line or API tools, DM Station GUI, or via the Mongo Express application

Mongo Express Database: dm > Collection: hammonds-25idtest-20220504-files

Viewing Collection: hammonds-25idtest-20220504-files

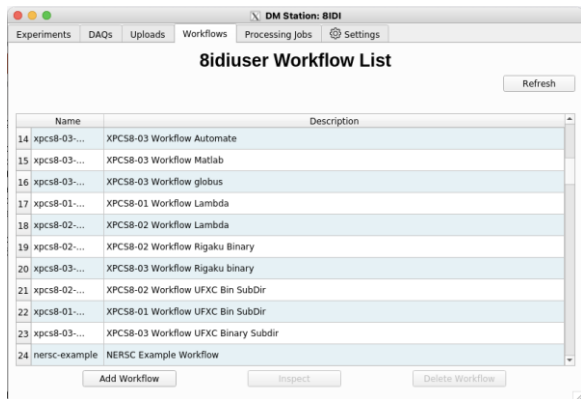
Simple Advanced

Key Value String Find

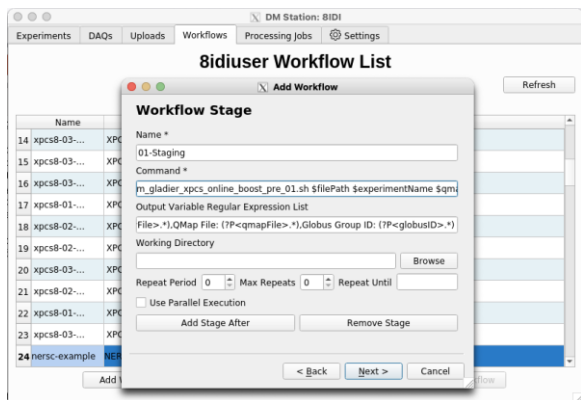
First Prev Next Last

_id	md5Sum	fileSize	fileProcessingTime	fileProcessingTimestamp	fileCreationTime	fileCreationTimestamp
62719c0541e17594b26abe6b	91817774e9c0b041a1d891ad4250831c	16540	1651612677.687332	2022/05/03 16:17:57 CDT	1651086103	2022/04/27 14:01:43 CDT
62719c0541e17594b26abe6c	d905d561d8773f7cebdfc17f2d120e03	32862	1651612677.7097344	2022/05/03 16:17:57 CDT	1651086103	2022/04/27 14:01:43 CDT
62719c0541e17594b26abe6d	9b07815839f8bab87409dbf0e0abde0	21556	1651612677.7267165	2022/05/03 16:17:57 CDT	1651086103	2022/04/27 14:01:43 CDT

# Station Services: Workflow Engine



- Processing Service provides support for managing user-defined workflows, as well as for submitting and monitoring processing jobs based on those workflows
- A DM workflow is a collection of processing steps
- Processing Service can be used standalone, or together with other DM Station services in support of fully automated beamline data acquisition and processing pipelines

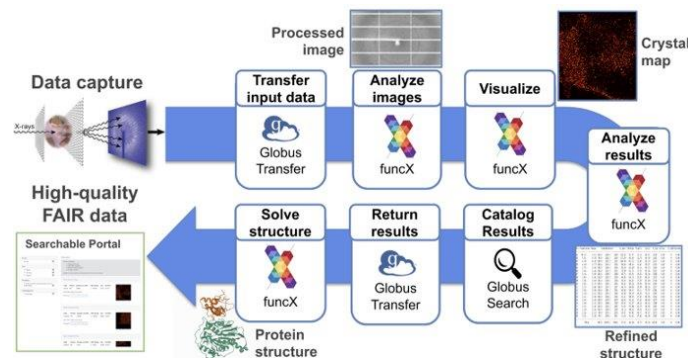


# Connecting with ALCF and Data Portals

- Data Management workflow engine used with the gladier toolkit to process x-ray photon correlation spectroscopy data using the Argonne Leadership Computing Facility in near real-time and publish to the ALCF Community Data Co-Op data portal

**ALCF Community Data Co-Op**  
Providing Researchers Data Sharing Capabilities

<b>APS 2D XRF</b> X-Ray fluorescence imaging for a variety of applications Private <a href="#">Search This Project</a>	<b>APS HEDM</b> High-Energy Diffraction Microscopy (HEDM) is a 3D technique which resolves the structures and strains of individual grains within bulk polycrystalline materials. Private <a href="#">Search This Project</a>	<b>APS Ptychography</b> A computational method of microscopic imaging by processing many coherent interference patterns Private <a href="#">Search This Project</a>	<b>APS XPCS</b> X-ray Photon Correlation Spectroscopy (XPCS) is a technique to study dynamics in materials at nanoscale by identifying correlations in time series of area detector images Private <a href="#">Search This Project</a>
<b>DLHub</b> A multi-tenant system that provides both model repository and serving capabilities with a focus on science applications Public Data <a href="#">Search This Project</a>	<b>Kanzus Beamline Chip Analysis</b> Synchrotron serial crystallography for the study of protein and enzyme dynamic processes Private <a href="#">Search This Project</a>	<b>Neurocartography</b> Large volume reconstructions of the fine structure of the nervous system Search Only <a href="#">Search This Project</a>	<b>The Materials Data Facility</b> A simple way to publish, discover, and access materials datasets Public Data <a href="#">Search This Project</a>
<b>X-ray Science Division Imaging</b> The IMG group designs, supports, and operates state-of-the-art x-ray			



Chard, Saint, Kelly, Ananthakrishnan, Chard, Skluzacek, Wagner, Narayanan, Sherrell, Schwarz, Blaiszik, Foster, "Gladier: An Architecture to Enable Modular Automation of Data Capture, Storage, and Analysis at Experimental Facilities," DOE Data Days 2020.

# Future Enhancements

- Streaming data directly from detectors to storage to decrease the transfer time as data rates and volumes continue to increase
- Workflows are being developed which publish to common data portals for visualizing results
- Interfacing with the tape archives of the Argonne Leadership Computing Facility will allow more data to be stored for longer periods.



**Thank you for your time**



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