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Managing Experiment Data with Ease at the Advanced Photon Source

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September 20, 2022

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

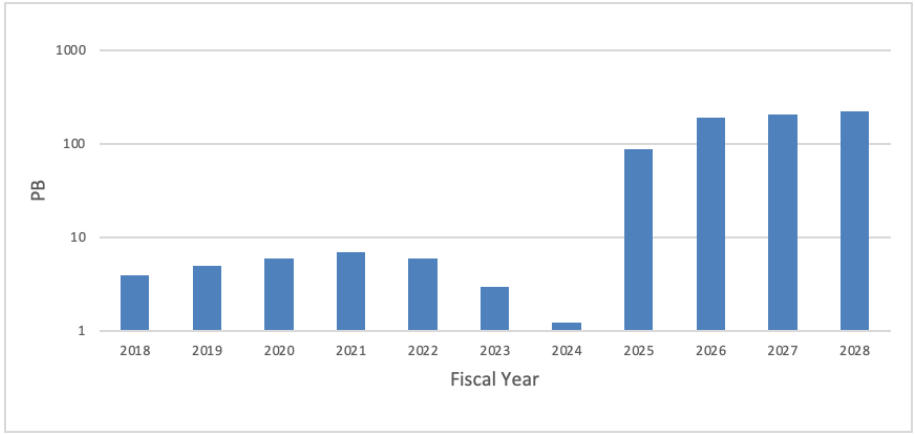
Advanced Photon Source (APS) at Argonne National Laboratory

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

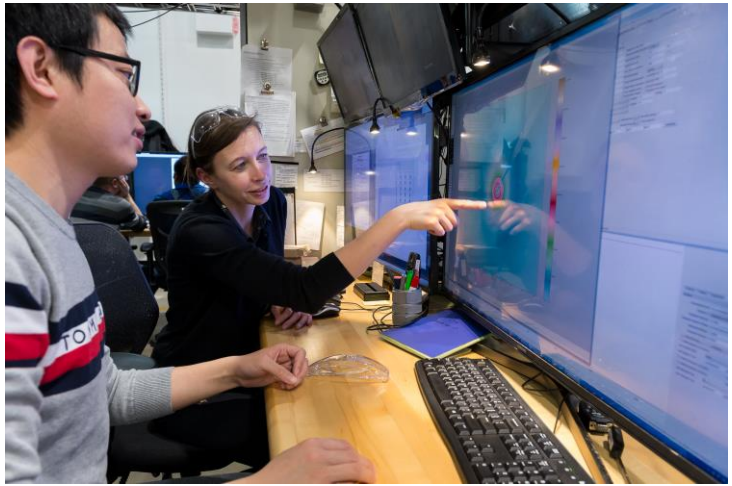
- In April of 2023, the APS will undergo a massive upgrade that will replace the current electron storage ring
- Once the upgraded APS storage ring and beamlines are commissioned and brought into operation, it is estimated that the volume of data generated at the APS will increase by at least two orders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

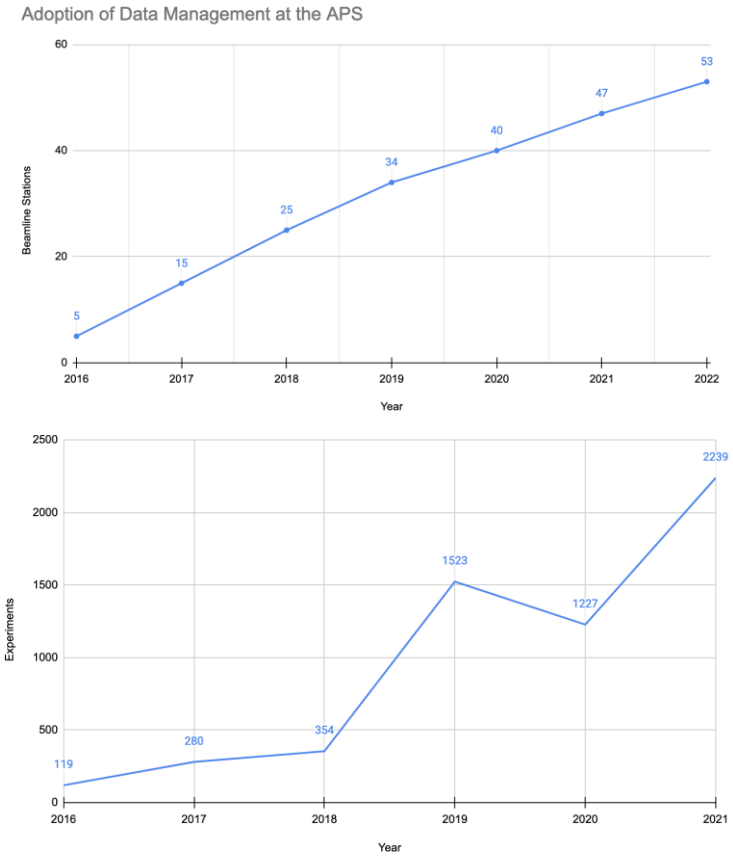
- Beamlines have multiple experiment techniques, types of detectors, data rates, data formats, operating systems, and processing workflows
- Users come from different research institutions, universities, and industries, and must be able to access their data after leaving the facility
- Users access data 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.



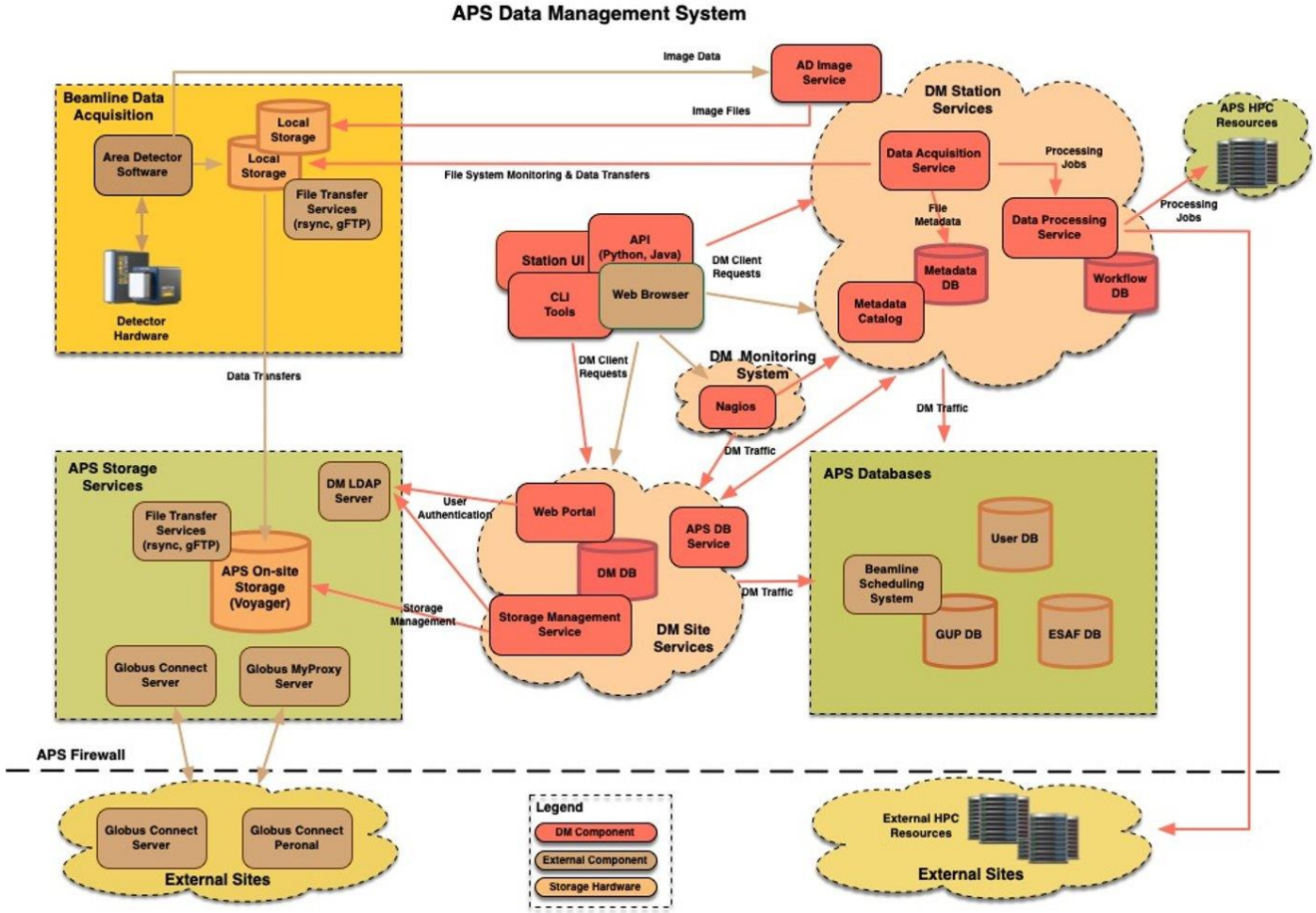
The Data Management System at the APS

- 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

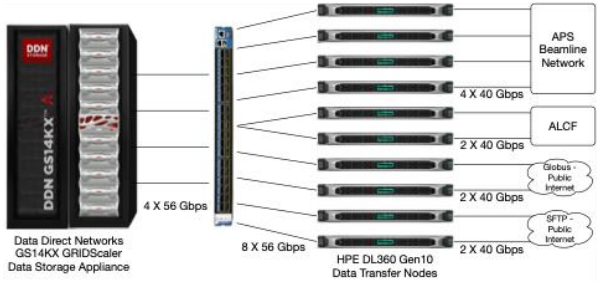
Impact of the Data Management System



- 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



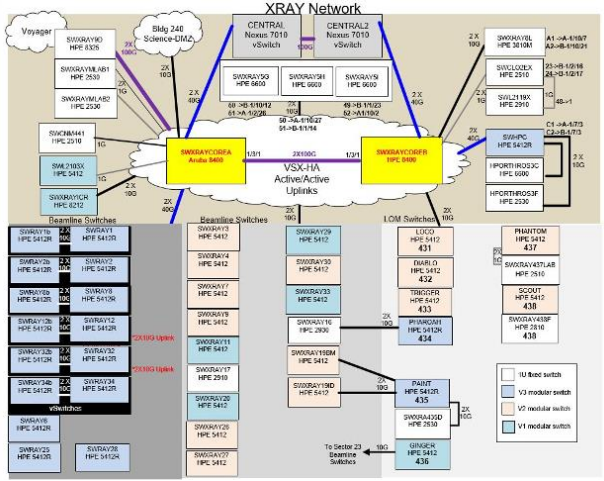
Infrastructure

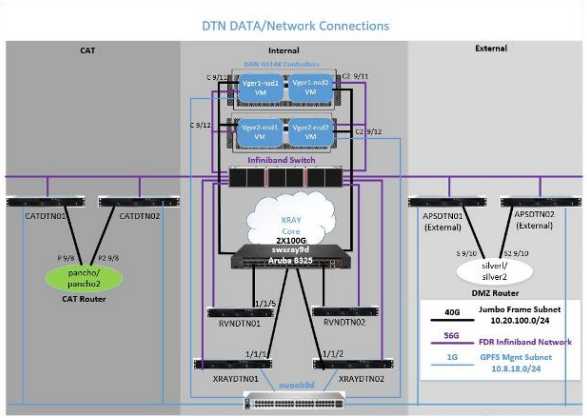


HPE ProLiant c7000 Enclosure

NetApp FAS 8200

HPE 3Par Family





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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

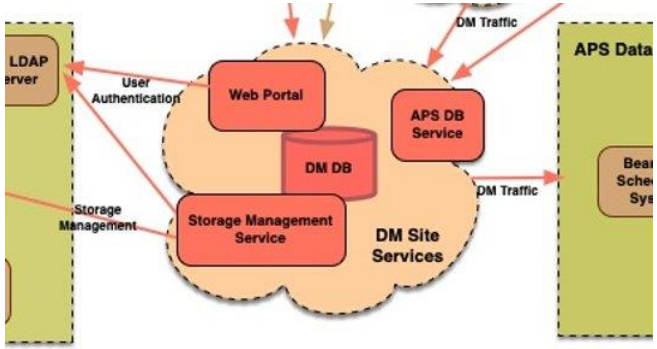
- GridScaler GS14KX file storage appliance, 6PB storage
- 8 Data Transfer Nodes: 1 Intel Xeon 6144 3.5GHz CPU, 128GB RAM, 40 Gbps ethernet link, 56 Gbps Infiniband, 2 x 400GB SSD drives (mirrored)

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



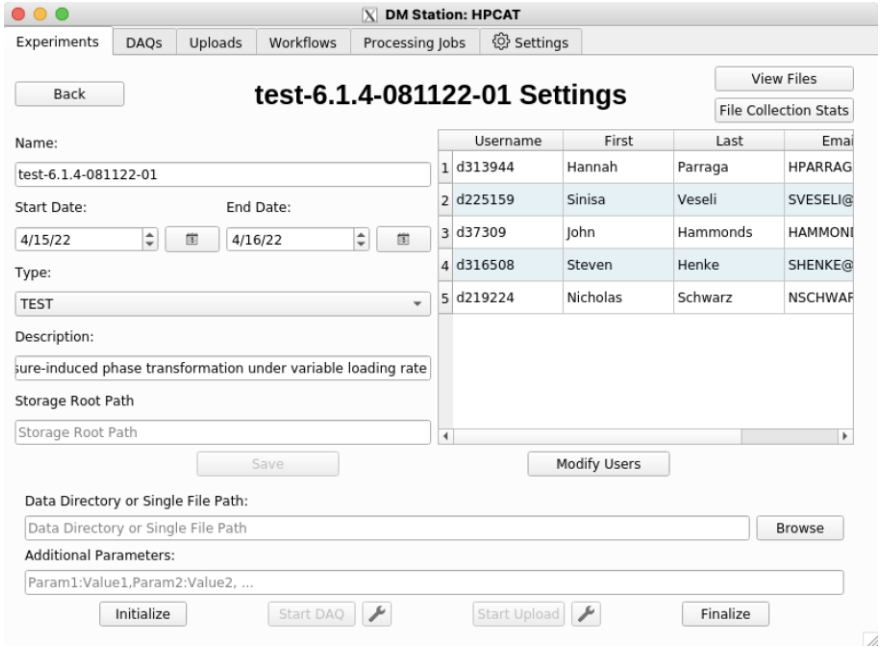
- APS DB Service (Python, REST)
  - Enables easy access to ESAF and GUP information
- Automated utilities for synchronizing DM user information with APS User Database

Monitoring

- 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

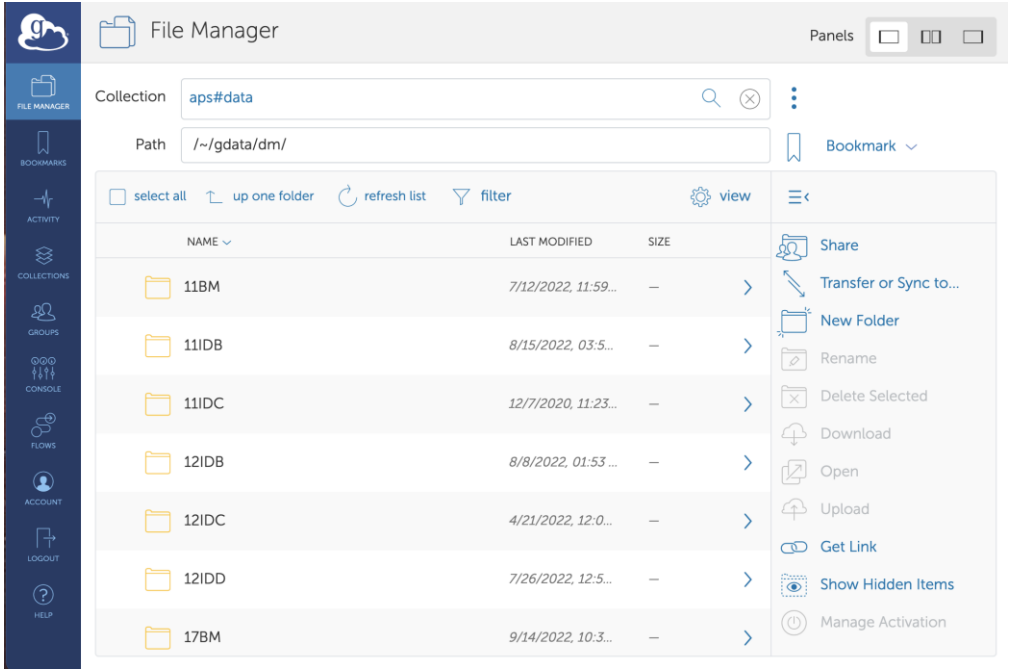
User Interfaces

- 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



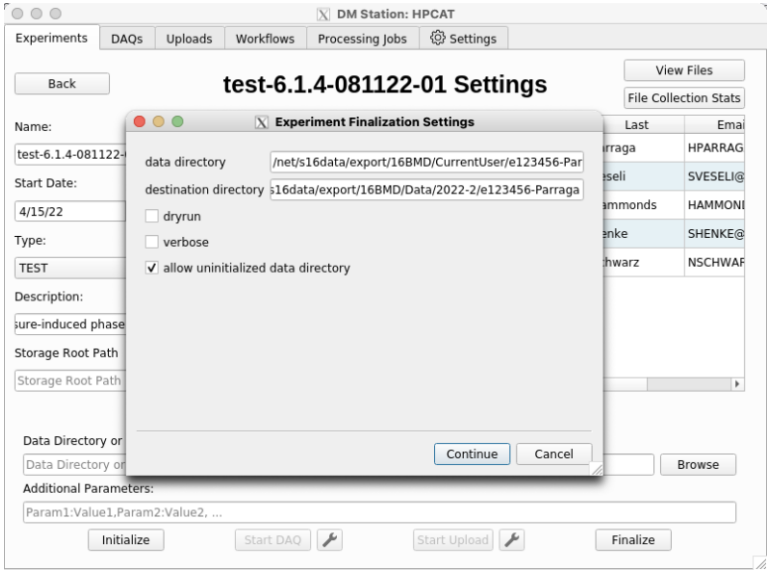
Data Access

- 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

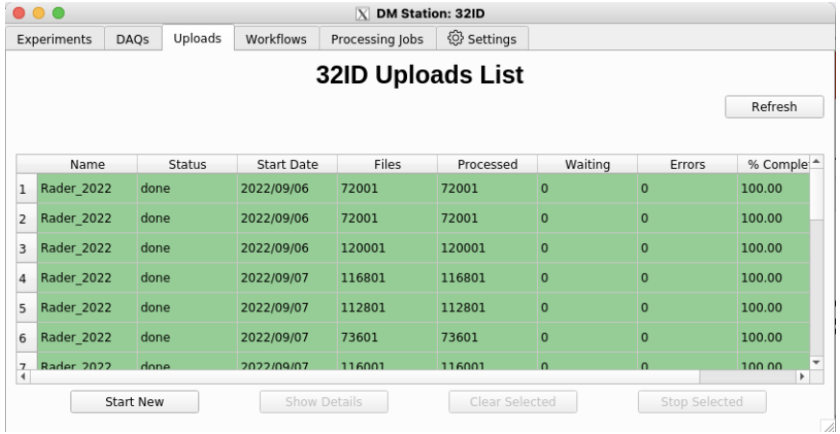
- Experiment data directories on local beamline machines can be "initialized" and "finalized"
- File permissions and access control lists can be set so that only the beamline administrator or allowed user group has access to the data local after the experiment is complete.



Station Services: DAQ Service

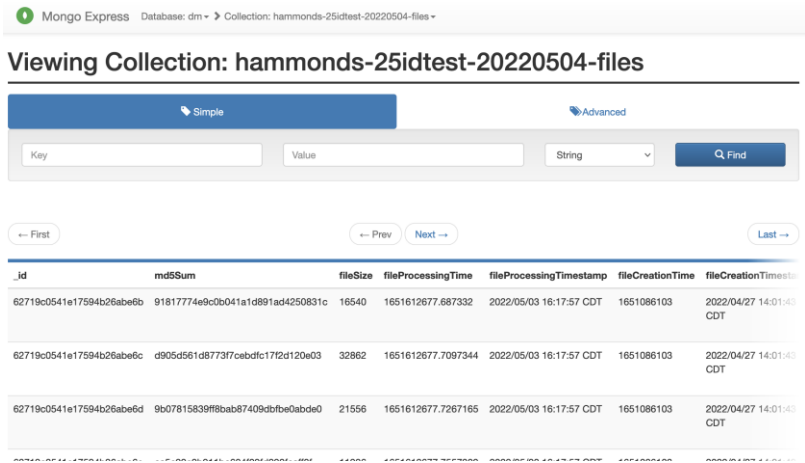
- Each beamline deployment (“DM Station”) includes several Python services accessible via REST interfaces: DAQ Service, Metadata Catalog and Processing Service

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

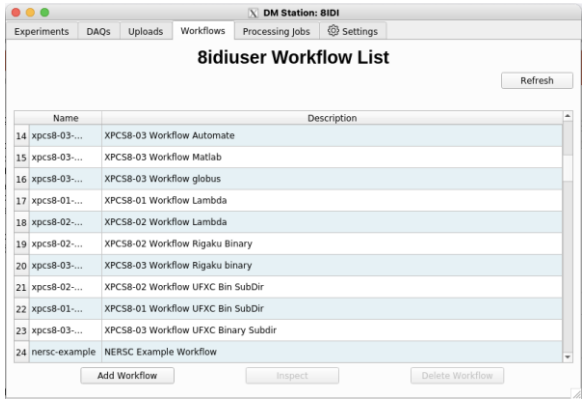


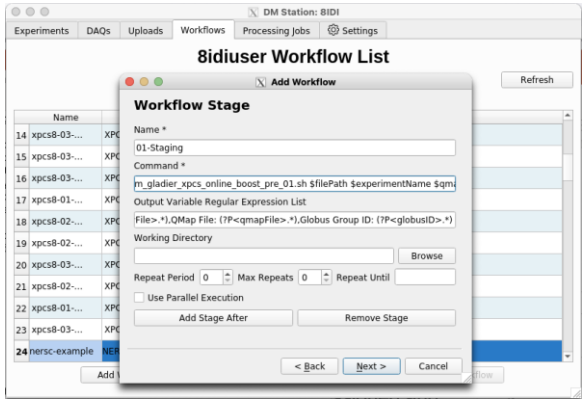
Station Services: Metadata Catalog

- 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



Station Services: Workflow Engine

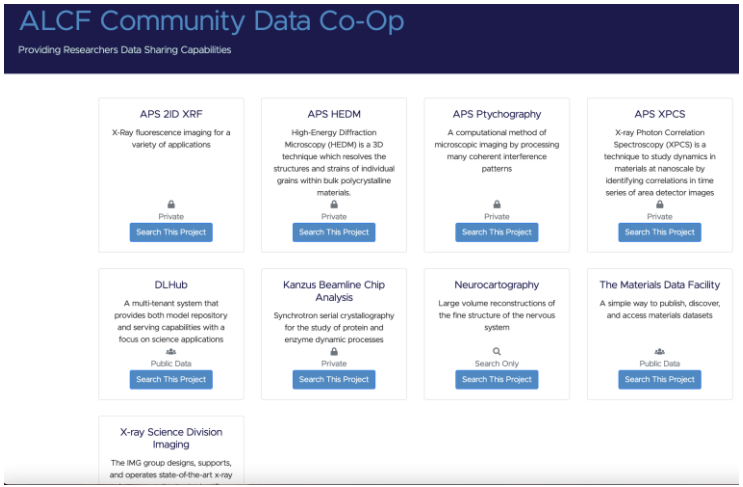


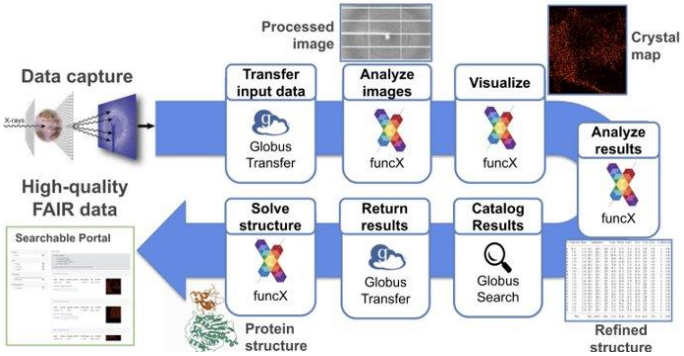


- Processing Service provides support for managing user-defined workflows, as well as for submitting and monitoring processing jobs based on those workflows
- A DM workflow is a collection of processing steps
- Processing Service can be used standalone, or together with other DM Station services in support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





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.

https://gladier.readthedocs.io/en/latest/gladier/overview.html

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

This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357. This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357.

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