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AUTOMATING SCIENTIFIC INSIGHTS AT THE ADVANCED PHOTON SOURCE

HIGH-PERFORMANCE WORKFLOWS FOR ANALYZING EXPERIMENTAL DATA

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OVERVIEW

Engineers at the Advanced Photon Source are creating automated data processing pipelines leveraging high performance computing to address increasing data needs and enable scientific discovery.

X-RAY LIGHT SOURCES

Indispensable tools in the exploration of matter

- Wavelengths of the emitted photons are similar to the atomic spacing of materials and biological cells
- Advanced Photon Source is one of 5 scientific user facilities 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

OBJECTIVE

Enable facility users to gain **meaningful scientific insights** from their experiments as quickly as possible by transforming raw X-ray detector data with some software appropriate for the experiment type (while **minimizing the burden of data processing** on the user).

SCALE OF THE PROBLEM

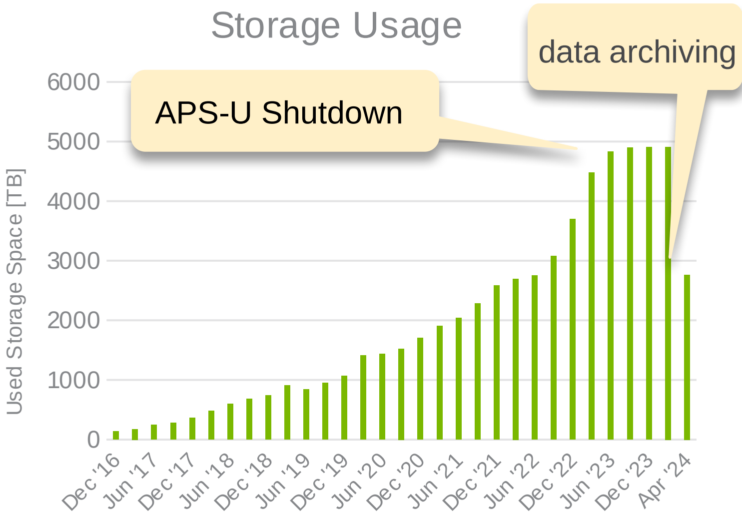
Multiple order-of-magnitude increase in demand for computing resources

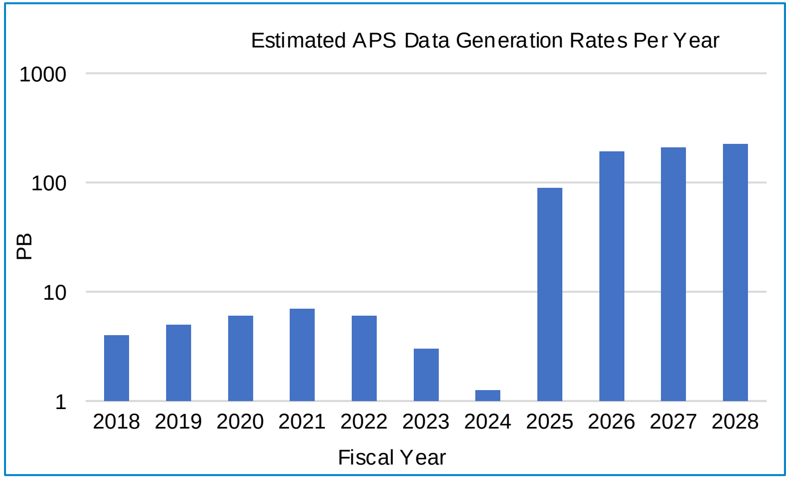
Over the past decade the APS has

- Created over 9000 experiments in the Data Management database
- Used 4.9PB of storage space

Over the next decade the APS will

- Generate 100s of petabytes (PBs) of raw data per year
- Require 10s of petaflop/s of on-demand computing power





REQUIREMENTS

Process experiment data…

Automatically with data collection

When a user triggers

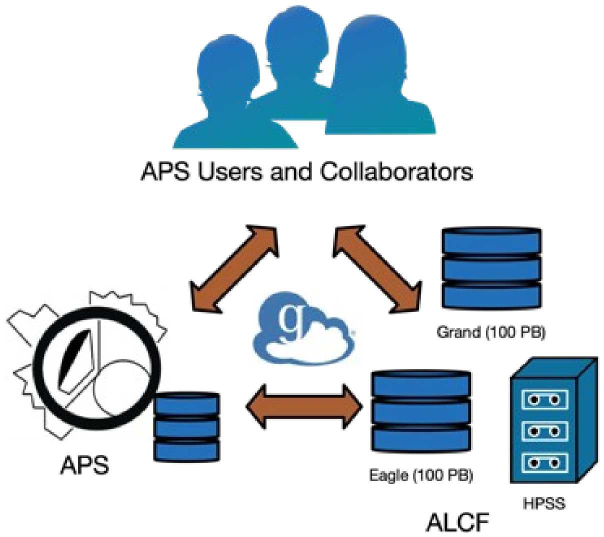
In different places

With a variety of software packages

THE APS DATA MANAGEMENT SYSTEM

Facility-wide software and hardware system for managing data

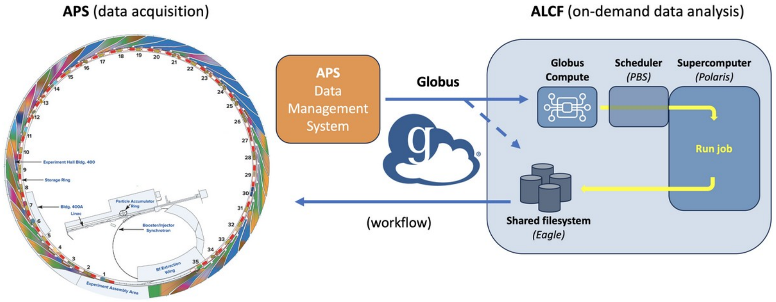
- Tools to automate **transfer** of data, manage storage **access** permissions, and **metadata** catalog
- Workflow tools automate data **processing** via plug-ins
  - Automated or user-initiated jobs
  - Flexible execution of any commands
  - Execute jobs locally or remotely
  - Integrated with Bluesky (beamline control software) and Globus

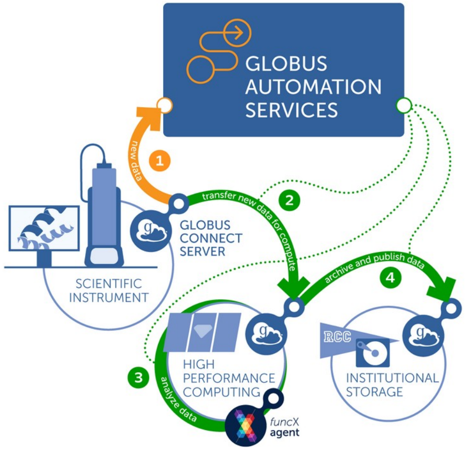


BRIDGING LARGE-SCALE FACILITIES

Advances from Leadership Computing Facilities and Globus

- Facility (ALCF/NERSC) collaboration means APS users do not need to navigate HPC
  - Priority “on-demand” queue for real time processing at ALCF
  - Service/collaboration accounts for beamlines
  - Computing allocations for APS
- Globus Compute
  - Function-as-a-service platform for remote job execution
  - Endpoints deployed at ALCF/NERSC
  - Secure access to data and compute resources





INTEGRATING CONTROLS WITH ANALYSIS

- Bluesky uses information on experiment conditions and where data is located to inform downstream analysis
- Bluesky plans use the APS Data Management API to launch workflows
- Users automatically get processed data when they run a Bluesky plan without extra effort

apstools / apstools / devices / aps_data_management.py

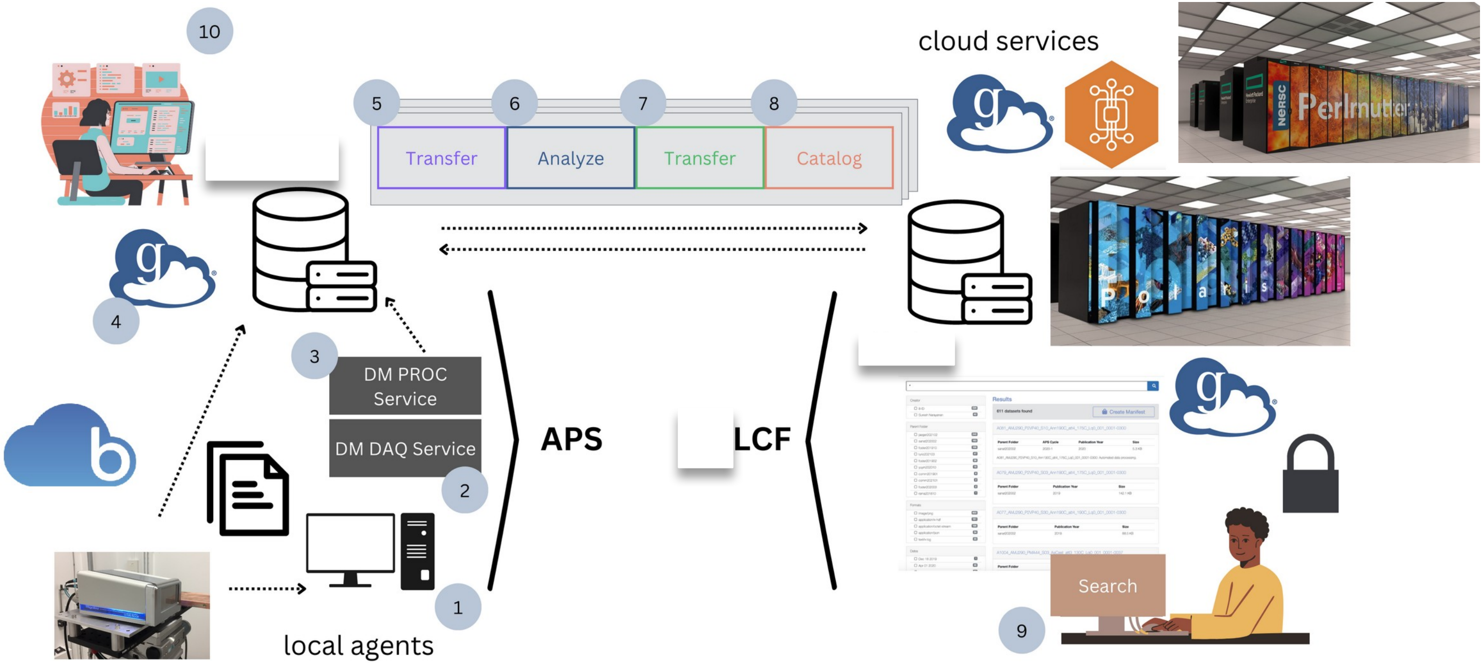
prjemian MNT #872

Code Blame 347 lines (287 loc) · 11.4 KB

```
"""
Connect with APS Data Management workflows.

Example::

    import bluesky
    from apstools.devices import DM_WorkflowConnector

    RE = bluesky.RunEngine()

    dm_workflow = DM_WorkflowConnector(name="dm_workflow", labels=["DM"])
    RE(
        dm_workflow.run_as_plan(
            workflow="example-01",
            filePath="/home/beams/S1IDTEST/
        )
    )
```

Bluesky tools for APS by Peter Jemian and Eric Codrea

DATA LIFE CYCLE



1. Users fill form about experiment
2. Experiment database info populated from form and directory created in central storage
3. Start monitor for files
4. Acquire data and writes metadata
5. Transfer files to storage
6. Select workflow and arguments
7. Data processed locally or with HPC
8. Result published to portal
9. After time, data archived to tape

DATA PROCESSING

Standardized processing for common X-ray techniques

= operational
= in progress

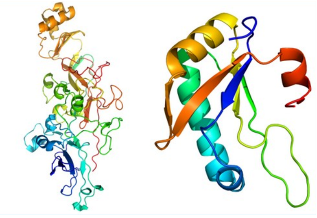
High-energy Diffraction Microscopy
1ID, 20ID
https://github.com/marinerhemant/MIDAS

Wide Angle and Small Angle X-ray Scattering
1ID, 20ID, 12ID
https://github.com/marinerhemant/MIDAS

X-ray Photon Correlation Spectroscopy
8ID, 9ID
https://github.com/AdvancedPhotonSource/boost_corr

Crystallography
23ID
https://www.gmca.aps.anl.gov/

Laue Micro-diffraction
34ID
Prince *et al.*, 2023

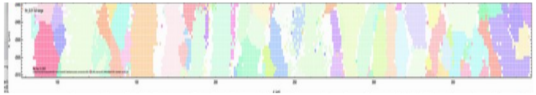


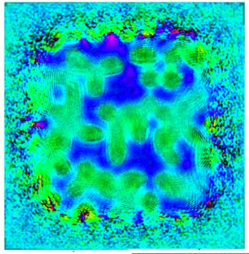
Ptychography
2ID, 4ID, 9ID, 12ID,19ID, 26ID, 28ID, 31ID, 33ID
https://github.com/AdvancedPhotonSource/ptychodus

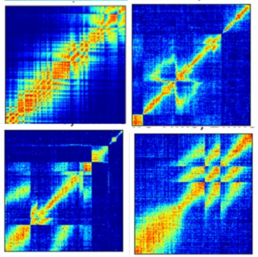
Grazing Incidence X-ray Scattering
9ID
Werzer *et al.*, 2024

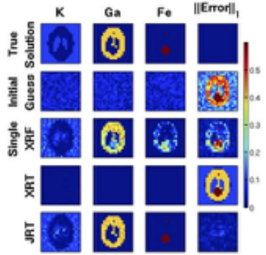
Tomography/Laminography
1ID, 2ID, 2BM, 7BM, 19ID, 20ID, 31ID, 32ID
https://github.com/tomography/tomocupy/

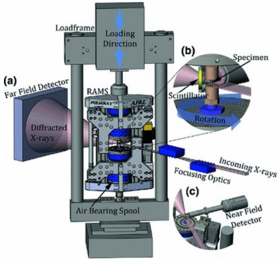
X-ray Fluorescence Microscopy
2ID, 4ID, 12ID, 19ID, 33ID
https://github.com/AdvancedPhotonSource/XRF-Maps











MULTI-TIERED APPROACH

Utilize local and remote resources

High-end compute resources

- Large data processing tasks, ML training, post-processing, and data refinement

Local compute resources

- Perform pre-analysis/data reduction
  - Compression and running ML models
  - Quality control and experiment steering
- May include a GPU workstation at a beamline or the APS computing cluster

Argonne Leadership Computing Facility (ALCF)

Polaris
~44 PFLOP/s

Aurora
> 1 EXAFLOP/s

~4 PFLOP/s of Polaris is prioritized for prototype on-demand use by experimental and observational facilities; when Aurora is in User operations, all of Polaris will be prioritized for on-demand use

Synergy
Planning is underway for the next generation on-demand system prioritized for experimental and observational facilities

Next Generation Supercomputer
Planning is underway for the next generation leadership class supercomputer

Argonne Laboratory Computing Resource Center (LCRC)

Improv
~2.51 PFLOP/s
825 nodes with 2 AMD EPYC CPUs each

Bebop
~1.75 PFLOP/s
672 nodes with 36 Intel Broadwell cores each

Swing
~925 TFLOP/s
48 NVIDIA A100s | 768 AMD EPYC cores

Advanced Photon Source (APS)

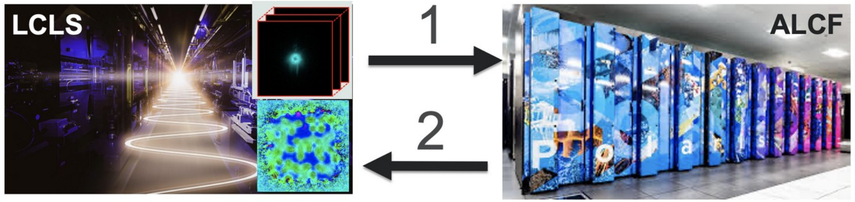
APS general purpose distributed-memory compute cluster
- ~20 TFLOP/s CPU cores

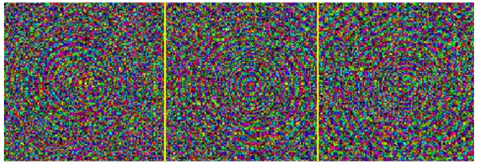
~50 High-Performance Computing Workstations
- Califone – 8 H100s
- Ecto – 8 RTX A6000s
- Refiner – 4 A100s
- Many others…

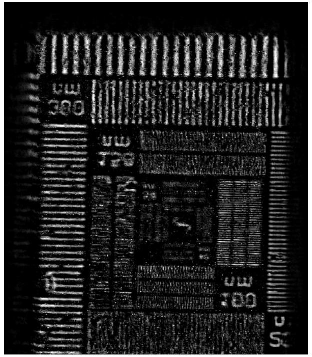
Edge Computing Devices
- 1 x NVIDIA Jetson AGX Orin
- 2 x NVIDIA BlueField-3 DPUs

PORTABLE CROSS-FACILITY WORKFLOWS FOR X-RAY PTYCHOGRAPHY

- Ptychography data volumes are expected to increase by *orders of magnitude* at leading X-ray research facilities due to next-generation upgrades
- Ptychography benefits from access to GPU computing resources
- We demonstrate cross-facility capabilities by deploying software at the **Linac Coherent Light Source (LCLS)**, packaging data and transferring it to **ALCF** for processing
- Used the ptychodus package







Vong *et al.*, 2024

FUTURE WORK

- Expand use of portals and integrate data management features into web pages
- Develop additional workflows and deploy at more beamlines
  - GSAS II, DIALS, laminoAlign and more
- Develop streaming workflows using PvaPy Streaming Framework

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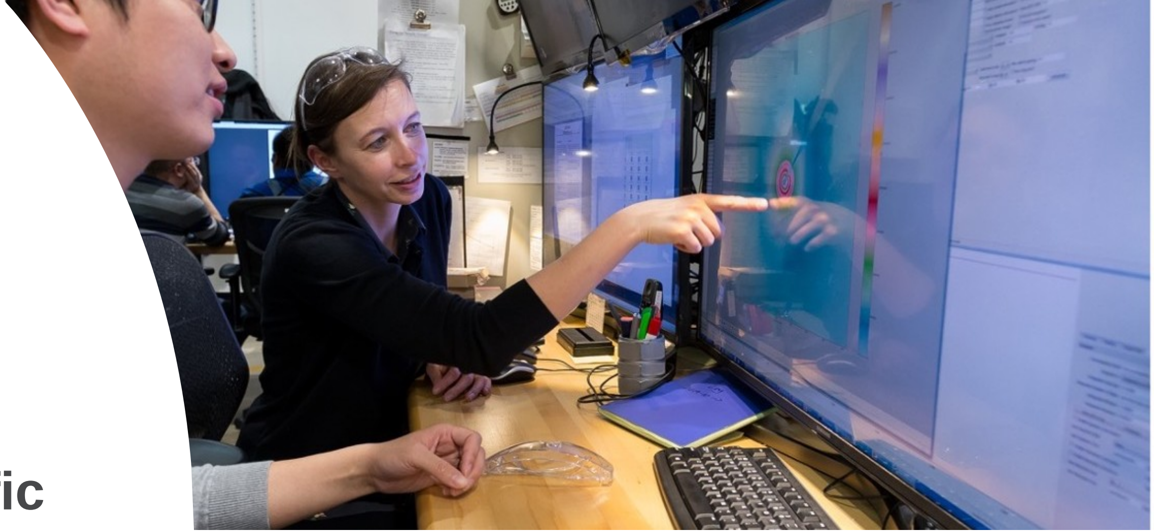
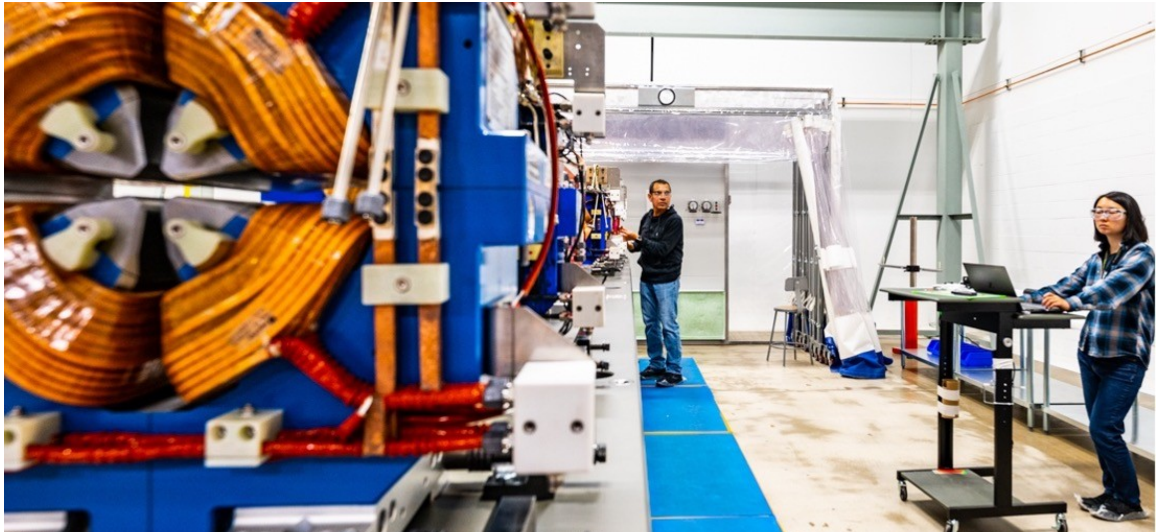
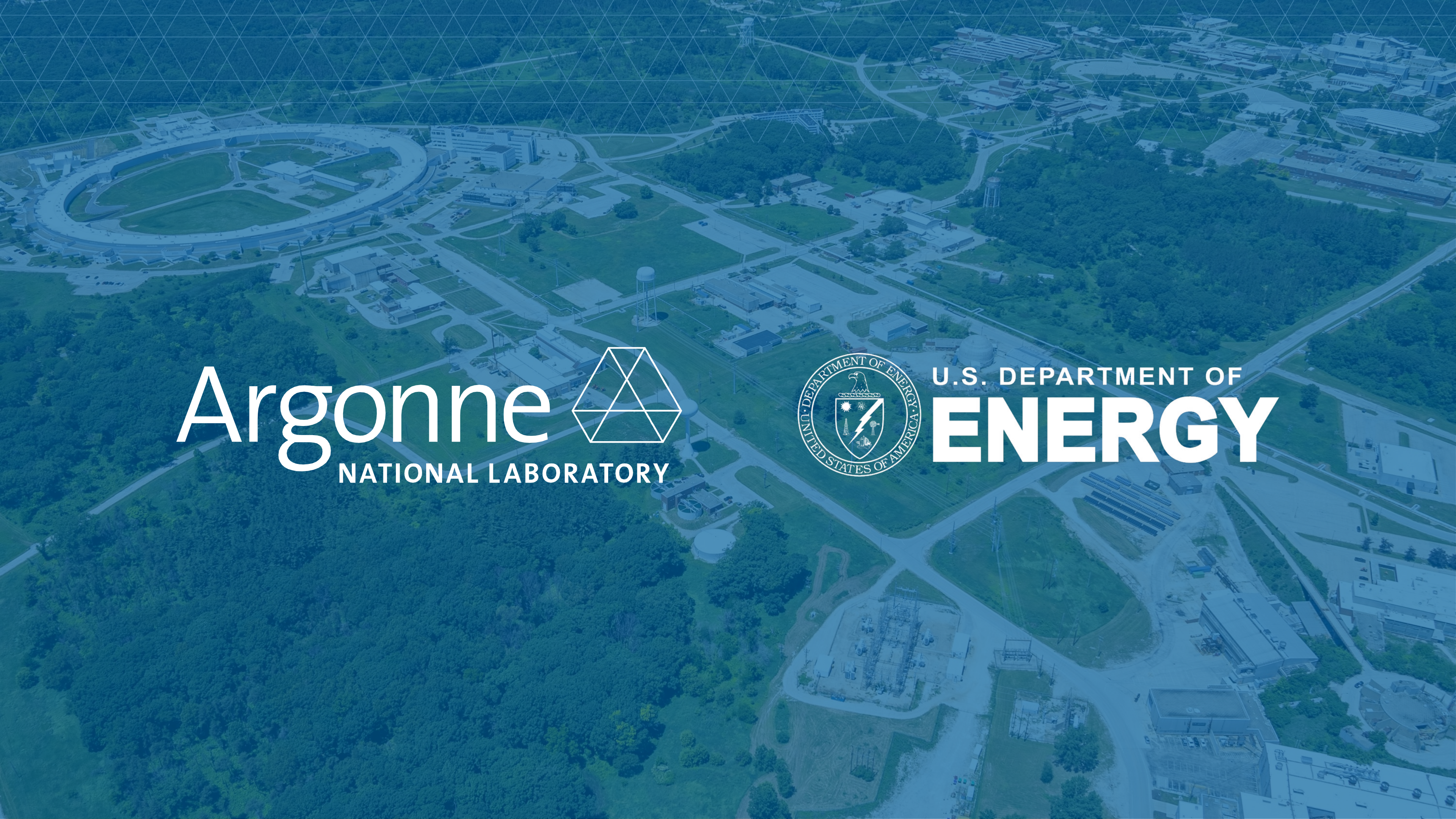
SUMMARY

The Advanced Photon Source is enabling scientific discovery and addressing increasing data needs by creating automated data processing pipelines leveraging high performance computing.



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