

# THE ADVANCED PHOTON SOURCE

## LEVERAGING ADVANCED COMPUTATIONAL RESOURCES FOR DATA ANALYSIS AND MANAGEMENT AT THE APS

Data are essential to the scientific discoveries enabled by the experimental techniques performed at the APS. The successful management of Big Data is of particular importance to current and future scientific productivity. The APS is teaming with other resources at Argonne to help with this challenge.

For instance, the APS has teamed with the Argonne Leadership Computing Facility (ALCF) and the Globus Services organization to help realize solutions for its Big Data challenges. The ALCF provides a 1.5-PB storage system for APS data. Data management software integrates beamline data workflows to transfer and catalog data. Access permissions are set so that researchers can download data at their home institutions using the Globus Online data transfer tool. The system is currently in use at many X-ray Science Division beamlines, and is being piloted by eight APS collaborative access teams.

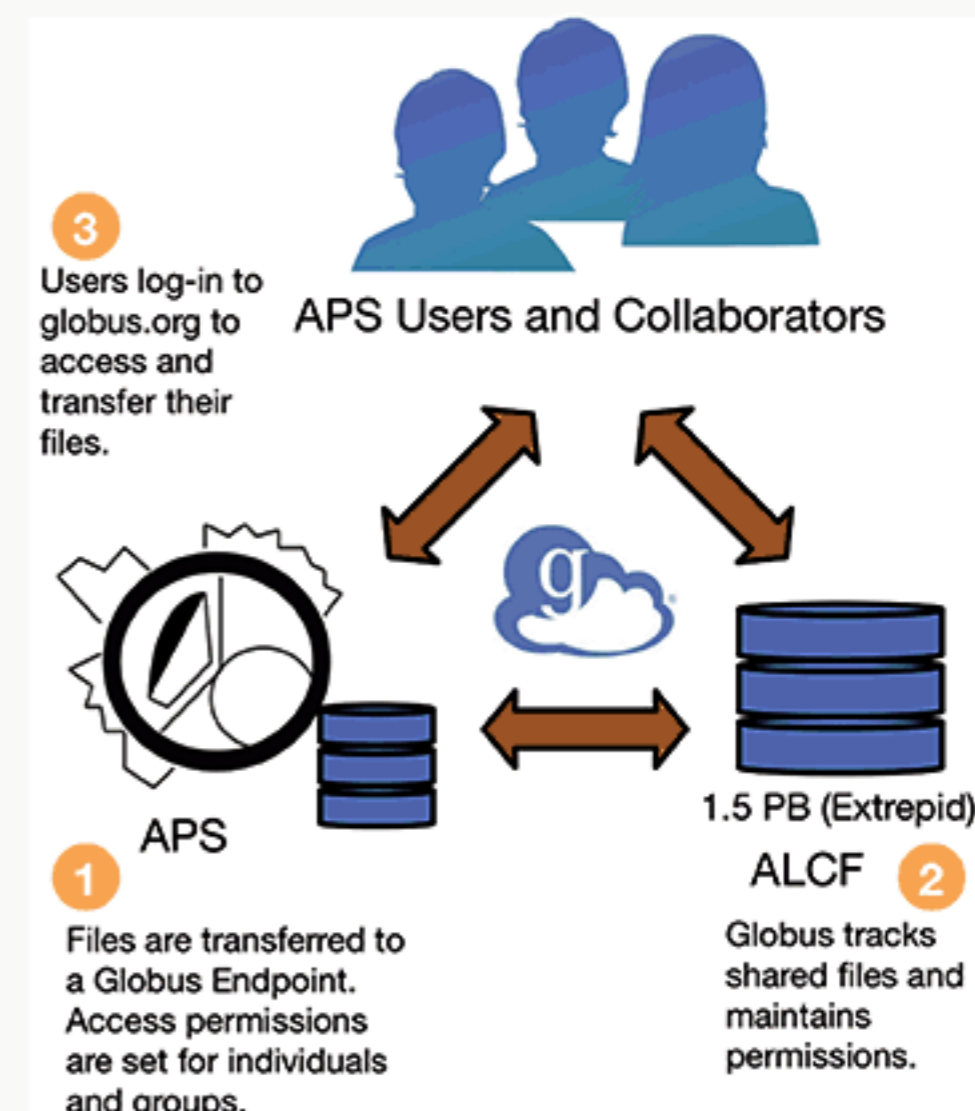
The APS has also teamed with the Argonne Computing, Environment, and Life Sciences Directorate to use Magellan, a virtualized computing resource located in the Theory and Computer Science (TCS) building. A workflow pipeline automatically transfers data from the APS to Magellan where Hadoop MapReduce-based autocorrelation routines are run. The whole process is completed shortly after data acquisition, typically in less than one minute. The faster turnaround time helps scientists make time-critical,

near real-time adjustments to experiments, enabling greater scientific discovery.

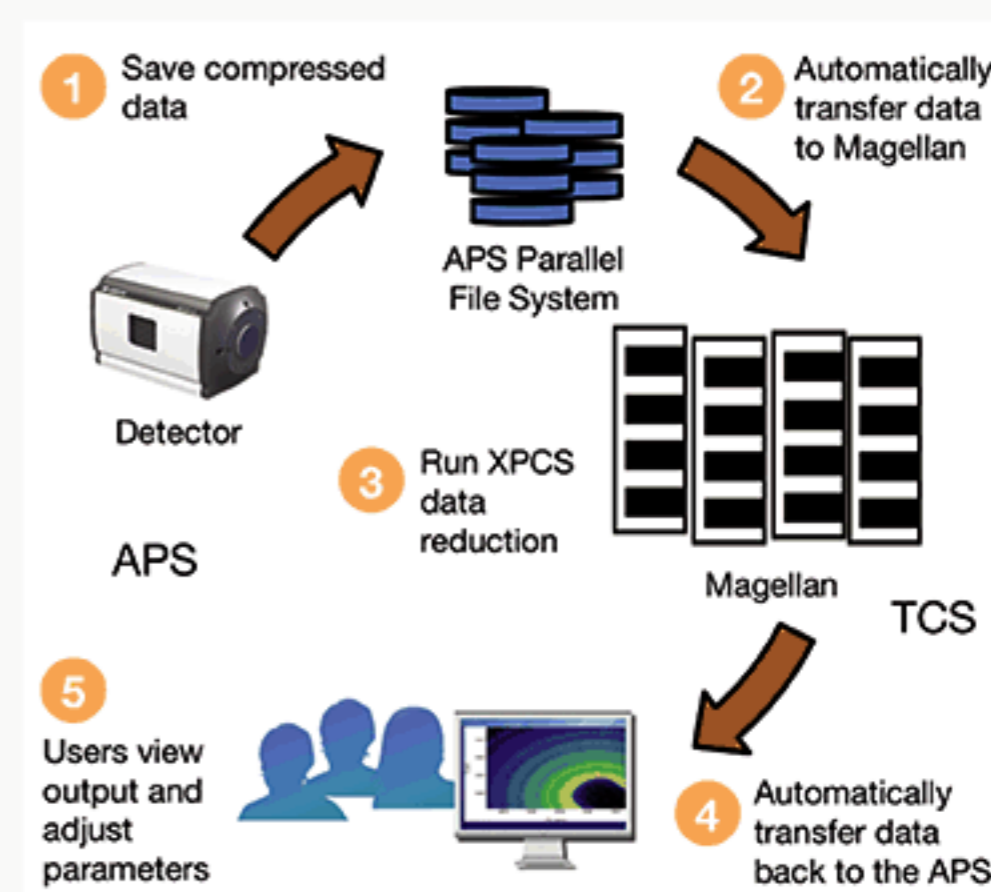
In collaboration with the Argonne Mathematics & Computer Science Division, the APS has developed a new high-performance elemental mapping toolkit for x-ray fluorescence microscopy beamlines. Given simultaneously captured fluorescence and transmission data, an optimization-based approach for joint inversion provides a simultaneous reconstruction of both the quantitative spatial distribution of all elements and the absorption effect in the sample.

PtychoLib, a parallel software library for real-time ptychographic phase retrieval, uses a hybrid parallel strategy to divide the computation between multiple GPUs, and then employs novel techniques to merge sub-datasets into a single complex amplitude image. Utilizing a 128-node GPU compute cluster at the ALCF connected to the APS via four 10-Gbps network links, the PtychoLib software is able to produce near real-time reconstructions. Together, these systems play a critical role in the analysis of data from many beamlines, now and in the future.

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Above: The Extrepid system housed in an ALCF computing center provides 1.5-PB of storage space for the APS. APS users and collaborators can access data using Globus Online. Below: XPCS integrated workflow pipeline depicting data flow from acquisition at APS 8-ID, to the TCS building for computation, and then back to the APS for visualization and interpretation.



### CALL FOR APS GENERAL-USER PROPOSALS




The Advanced Photon Source is open to experimenters who can benefit from the facility's high-brightness hard x-ray beams.

**General-user proposals for beam time during Run 2018-1 are due by Friday, October 27, 2017.**

Information on access to beam time at the APS is at [http://www.aps.anl.gov/Users/apply\\_for\\_beamtime.html](http://www.aps.anl.gov/Users/apply_for_beamtime.html) or contact Dr. Dennis Mills, [DMM@aps.anl.gov](mailto:DMM@aps.anl.gov), 630/252-5680.

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