REMOTE COLLABORATION VIA DISTRIBUTED HDF FILE ACCESS

Enabling collaborative, small accesses to large remote files in Python

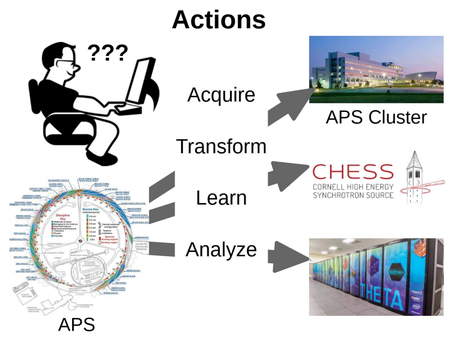
Justin M. Wozniak, Data Science and Learning Division, Argonne National Laboratory
Raymond Osborn, Materials Science Division, Argonne National Laboratory

ABSTRACT

Cross-institutional data sharing is still a challenging problem for the large datasets collected at the Advanced Photon Source (APS). Sector 6 at the APS routinely collects single-crystal x-ray diffraction data at a rate of several terabytes per day, which is streamed for automated data reduction in local file stores. Such large data volumes make it challenging to collaborate on data analysis with remote collaborators, without the inefficiencies of transferring full datasets.

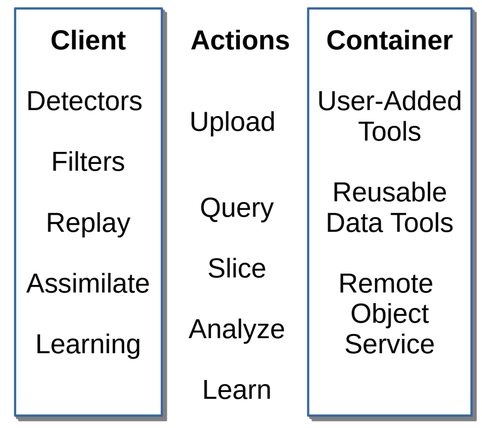
In our approach, users are presented with a unified view accessible to all collaborators, which is populated on-demand with experimental data and/or theoretical simulations from multiple sources, and synchronized with distributed remote locations (cloud, exascale computing facilities) as needed. From the user perspective, this will have three advantages: (1) accelerated analysis and learning pipelines due to reduced data transfer overheads; (2) improved integration of data analysis and advanced modeling, and (3) increased productivity due to less management overhead and development overhead.

MOTIVATION



Multiple stages in data analysis workflow distributed across multiple computing sites, each with differing processing and I/O capabilities. Typically, whole data sets are copied in bulk, incurring complexity and inefficiencies.

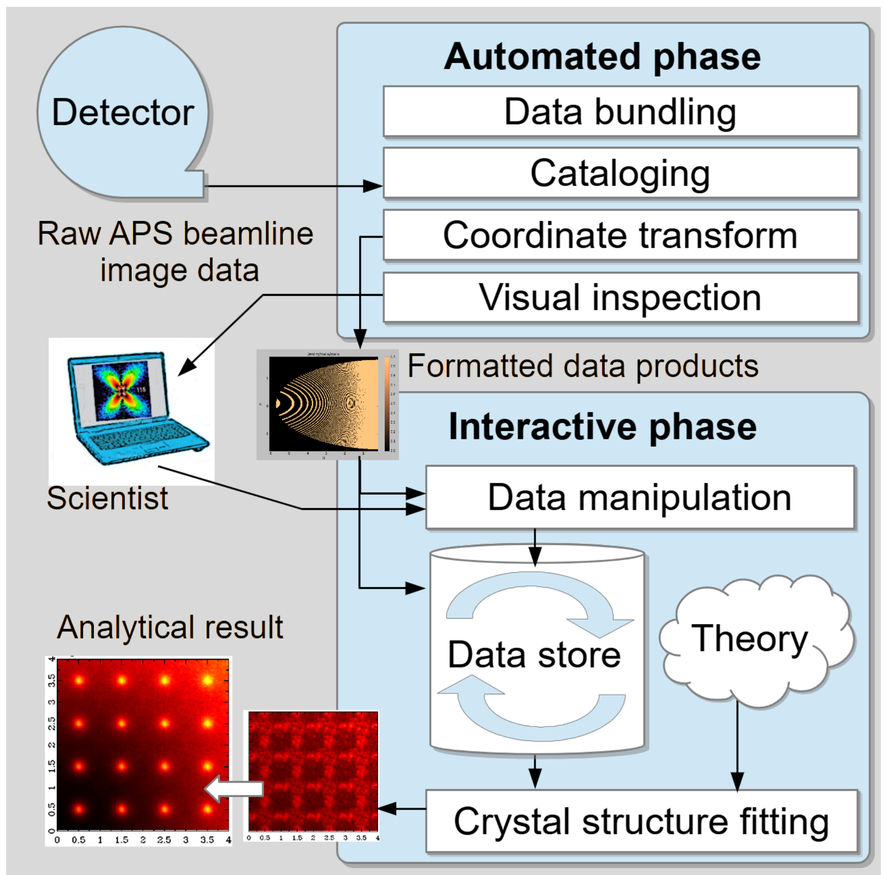
METHODS



Multiple stages in data analysis workflow supported by remote data tools, including serving Pythonic objects for learning from small slices of large data.

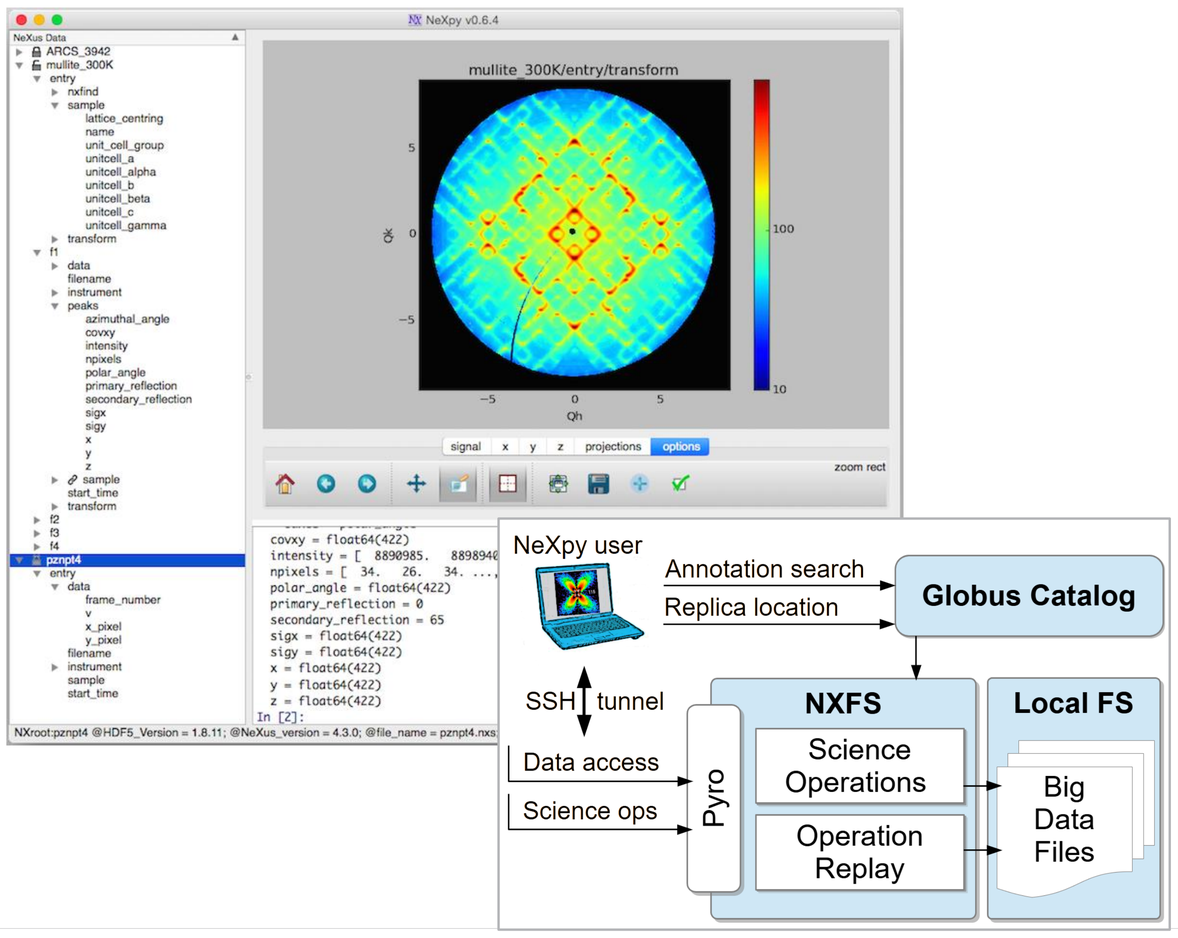
SMALL ACCESSES TO LARGE DATA

- There is a need to be able to collaborate with remote users performing visualization, lightweight analysis, and small data modification on these datasets, tasks for which the full dataset is not needed. Thus, we desire to create a system in which it is possible to enable remote data slicing and selection.
- Want to be able to perform slicing, visualization, analysis, and learning on remote data.



USING THE HDF OBJECT INTERFACE

- The HDF interface allows for the possibility of lightweight data access, at least at the interface level. We are prototyping this approach using the a Pyro wrapper around HDF, a distributed service that can be hosted on an institutional cluster or commercial cloud and accessed by a remote client. This proposed solution integrates with existing analysis routines and visualization tools such as NeXpy.



CONCLUSIONS

- Our approach is to develop a toolkit of learning and analysis-ready Python libraries that can be integrated into workflows by users from a broad range of disciplines.
- Enhanced data analysis and learning will be enabled through extensions to a remote object toolkit which provides a familiar numerical interface, and optimizable aggregated data pipelines for learning frameworks.
- We want to enable the orchestration of remote data sources, selecting from available datasets, providing high level indexing and query support to extract, group and present the data from multiple data services.

SOFTWARE CAPABILITIES

- We have made widespread use of HDF5 external links in the prototype as a way of separating the raw data, that should be immutable and protected from corruption, and the higher level metadata both from the experiment and added through the pipeline.
- This prototype has been successfully demonstrated at both the APS and CHESS, and will soon be tested for joint analyses of diffuse scattering at APS and the Spallation Neutron Source. This project should be of use in encouraging interfacility cooperation through the standardization of remote data access procedures, and, potentially, in the design of remote data facilities.

REFERENCES

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- **Data object distribution for experimental science pipelines.** Justin M. Wozniak, Ray Osborn, and Jacob Ruff. ASCR Workshop on the Management and Storage of Scientific Data 2022.

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30” X 40” HOW CAN WE USE ENERGY FROM THE SUN TO MAKE FUELS?

Nature driven photochemical approaches to solar fuels

Sarah Soltau, Sunshine Silver, and Lisa Utschig, Chemical Sciences and Engineering Division, Sarah Soltau, Sunshine Silver, and Lisa Utschig, Chemical Sciences and Engineering Division, Sarah Soltau, Sunshine Silver, and Lisa Utschig, Chemical Sciences and Engineering Division

ABSTRACT

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METHODS

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NEXT STEPS

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