Abstract

The productivity of researchers using synchrotron X-ray sources requires robust, easy-to-use software with state-of-the-art visualization and analysis methods for ever more complex and larger data sets.

This project is integrating and improving existing analysis methods for multiple synchrotron X-ray techniques into the open source and extensible Larch X-ray Analysis framework based on the scientific Python stack.

The initial focus for this work is on the multi-modal data from X-ray microprobe beamlines, which can include X-ray imaging, fluorescence and absorption spectroscopy, and X-ray diffraction. The developments will provide a well-documented, well-supported, and extensible tools for researchers, students, and academics to visualize and analyze data from many synchrotron X-ray techniques.

Synchrotron X-ray Methods and Users

Synchrotrons are large user facilities providing very bright beams of X-rays for scientific research. Experiments are done at state-of-the-art beamlines, custom-built with ever-improving detectors and data collection methods. The Advanced Photon Source (see figure) at Argonne National Laboratory is the largest US synchrotron with ~ 60 simultaneous experiments and ~ 6000 user experiments per year. Data is large, complex, and heterogeneous.

Synchrotron work can include X-ray Scattering, Spectroscopy, and Imaging, each of which has many variations. Some of these have well-established analysis techniques and supported, user-friendly analysis programs, and some do not. New data collection modes and analysis methods are continually being developed.

Synchrotrons users come from a range of disciplines – material science, physics, biology, chemistry, geology. User productivity is often limited by visualization and analysis software to handle their particular kind of data. The facilities are not able to provide full support for all the needed tools. Typically, beamlines and expert user build these tools independently, and with little collaboration. We’re hoping to build a better way to build and support synchrotron X-ray analysis tools.

Analysis Tools for X-ray Spectroscopy

X-ray Absorption Spectroscopy (XAS) requires a synchrotron X-ray source but provides unique measures of chemical speciation and local atomic coordination. Full analysis needs ab initio calculations from solid-state physics. The procedures are well-understood, but can be complex.

First principle theoretical codes[1] and robust, CLI and GUI programs[2, 3] are well-supported and widely used in the XAS community. The Larch Framework builds on these tools, and will continue to support and improve state-of-the-art XAS analysis.

X-ray Fluorescence (XRF) Spectroscopy gives elemental abundances. XRF analysis is straightforward, but be complicated by non-linear detector effects and sparse data. Modern XRF analysis is most challenged by large data rates of several 100 spectra per second.

Larch includes XRF visualization (see figure) and crude analysis. We will improve and automate the XRF analysis methods, working in close collaboration with the developer of PyMCA[4].

Synchrotron XRF spectra can be collected in ~ 5 msec, and used to build elemental maps (left) of samples with spatial resolution of 1 μm or smaller. X-ray Diffraction (XRD) data can be collected at each pixel at ~ 50 msec per pixel.

Datasets with XRF spectra at each pixel can be several Gb / hour. With XRD patterns at each pixel, data rates are 100s of Gb / hour. Larch must provide tools to visualize and analyze these datasets for novice users from many scientific domains.

The Larch Framework

Larch builds X-ray analysis tools on top of the open source and well-supported scientific Python stack. It provides a domain-specific interactive session and simple plugin mechanism with all the necessary functionality for basic scientific data analysis:

- all data are Python objects, any Python modules can be used.
- complex numbers, multi-dimensional arrays (numpy), hashes, etc.
- loops, conditionals, error handling, user-defined functions.
- high-level plotting, image display.
- robust non-linear fitting, statistical tools.
- support for reading data from HDF5, SQL, (Globus soon!).
- standalone GUI apps for dedicated analysis tasks.
- accessible as plain python library.
- remote sessions via XML-RPC.

This flexibility and access to modern data formats allows us to apply proven algorithms to ever more complex, multi-modal datasets such as combined X-ray Fluorescence and Diffraction measurements.

Adding new visualization and analysis procedures has never been easier. We are starting to see “non-programmer” scientists experiment with analysis codes and contribute work that others can use, getting credit, but without having to package or distribute themselves.

User Communities and Outreach

We are building on the community from the earlier IFEFFIT tools, so have an existing and active mailing list, and annual short courses, and built-in user base for X-ray Absorption Spectroscopy. We are expanding this to synchrotron users of XRF Mapping and Analysis, and also to X-ray Diffraction and Scattering.

Annual workshops (first one: April, 2016) will foster collaboration with other X-ray analysis experts and beamline scientists, identify development directions, and bring in new contributors and power users. We will continue to train new users in these analysis methods with a modern, flexible, and comprehensive framework.

References


NSF SI2 (SSI) Project #1450468  http://cars.uchicago.edu/xraylarch  newville@cars.uchicago.edu