A Cohesive Approach to XAS Data Collection, Analysis and Workflow

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Since the relatively recent establishment of a quantitative theoretical framework to describe Near Edge X-ray absorption phenomena in the mid 70's[1,2], the field of X-ray Absorption Spectroscopy has exploded. This multidisciplinary chemical analysis technique can be performed at some 50 synchrotron radiation user facilities worldwide. The technique's inherent elemental specificity and minimally invasive nature have meant that far from being a phenomenon reserved for the curious physicist, it has become a staple analytical technique used in diverse scientific fields such as materials science, soil science, geology, etc. As the application and user community continues to expand, it is increasingly important that best practices and data handling expertise are made easily accessible to researchers. The overarching goal is to facilitate the incorporation of this technique as part of broader multidisciplinary research programs. To this end we have created a web application for the dissemination and processing of data collected at the Spherical Grating Monochromator (SGM) beamline at the Canadian Light Source (CLS).

The data workflow moves as follows: upon acquisition the data collected at SGM-CLS is written into a NeXuS[4] formatted HDF5 file and placed on to an HDF Server[3]. This HDF REST server is in constant communication with the web-app which populates an SQL database with every scan collected at SGM. The web-app uses this database to create further abstract models/groupings determined by the metadata stored in the NeXuS file. These groupings are used facilitate the processing and reduction of data, tasks which are offloaded onto a calculation REST server hosted at the CLS.

The combination of the HDF REST and the calculation REST servers enable the web-app to deliver a streamlined data workflow from acquisition to processing through one cohesive interface. This method lessens the learning curve required of users in order to obtain their processed spectra. By its nature, this framework allows for built in data integrity; each step in the processing sequence, (be it simple averaging, or interpolation of slew scans) can be traced back to the raw acquired data and the operations performed in-between. As features are added, and practices improved it is done so centrally, making the redeployment of improvements in the application framework instantaneous.

The web-app at present, has become an integral part of data acquisition workflow at the SGM beamline. Since its launch in November 2017 the active daily usage has increased steadily by *ca.* one user for every research group visit. Features are being actively developed and deployed, and with them this centralized framework will further facilitate the employment of XAS as an important analytical technique for multidisciplinary research programs.

References:

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