Abridged Spectral Matrix Inversion – Fitting 25,000 Spectra Per Second

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Recent improvements in both detector and readout speed have led to a substantial increase in the volume of X-ray fluorescence imaging (XFI) data. This results in increased challenges when processing XFI data; both in terms of computational limitations as well as the real time required to fit the datasets and development of improved methods is therefore important.

In a digitized XFI spectra the signal of interest is contained across a very small number of bins. Condensing the spectrum to only those bins leads to a significant reduction in computational overhead placed on the fitting program, M-Blank.

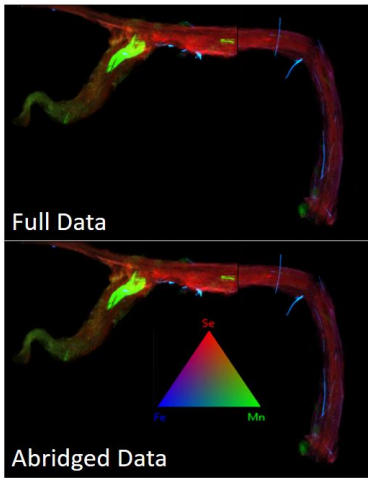

Figure 1: Fitted Astragalus images from the full data array and the abridged data array.

Figure 1 shows prototypical results presented previously demonstrating a negligible change between fits obtained from abridged and full datasets. As shown previously, to abridge the data and fit it to a series of modified Gaussians, the equations used for fitting are reduced in size by removing all channels that do not contain a value of a given percentage of the maximum for all equations being fit. Fig. 2A shows a series of normalized modified Gaussians with red lines indicating the points on the curves that correspond to the threshold being applied. Fig 2B is the same as Fig. 2A but with the area between the red dashed lines set to zeros. Fig. 2C shows the final equations after the area between the red lines is completely removed. Importantly, the corresponding channels from the raw XRF data are also removed prior to matrix inversion.

At last year's DXC, we presented this new conceptual approach to XFI data fitting called abridged spectral matrix inversion and presented preliminary test results obtained by inserting the functionality at the tail end of pre-existing fitting software package. This concept has been further refined from a theoretical concept demonstrated by inclusion of code introduced at the tail end of an existing software package, and the containing software package has been entirely rewritten around the concept allowing for the fitting of ~25,000 spectra per second. This year's talk will encompass a very thorough quantitative comparison between non-abridged and abridged datasets. The talk will be different from last years as last years was more conceptual and mathematical whereas this year it will be more data driven.

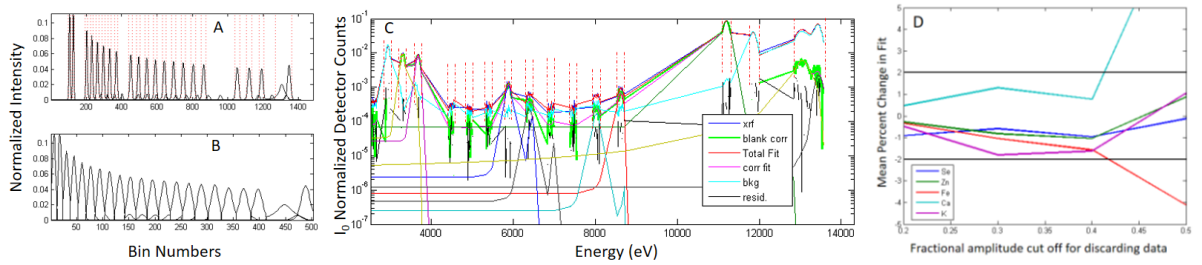

Figure 2: Abridged Data: The full equations (A) are abridged (B) by omitting all bins not between the red dashed lines. Likewise, the raw XRF data are abridged and fit to ultimately yield the fitted spectra (C). The mean percentage difference (D) between the abridged and full datasets using the full dataset as the baseline for comparison, shows less than a 2% deviation in quantified masses. The horizontal black lines mark ±2 percent.