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A novel computational method for X-ray fluorescence data and its deployment in the workflow of a beamline

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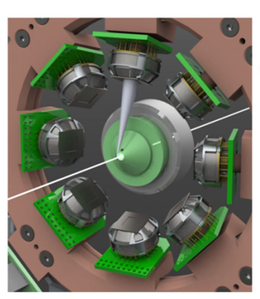
We present a computational method and the challenges for integrating it in the control system and workflow of a synchrotron beamline in operation.

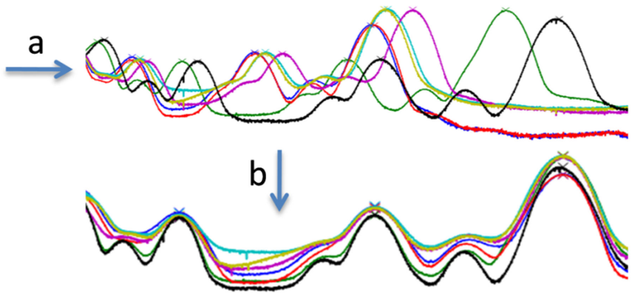
An important computational operation in a set of spectra is that of aligning them to a reference spectrum. In X-ray Fluorescence this is referred to as energy calibration and may be necessary for fitting low count acquisitions. Typically this is done in a linear manner and sometimes requires user feedback. Automated methods exist but are often focused to specific type of data. We have recently published [1] such a new automated method that is based on a non-linear approach and is specialised for XRF data. The initial application in two different multi-element detector systems in the beamline TwinMic (Elettra - Sincrotrone Trieste) yielded promising results.

We outline the introduction of the method and the software strategy we followed in order to integrate it to the workflow of an operating beamline. This should serve as a case study where a novel computational method is introduced to the standard information workflow of a lab. The underlining technology is based on “DonkiOrchestra: a scalable system for data collection and experiment management based on ZeroMQ distributed messaging” (NOBUGS2016 presentation).

Multi element XRF detectors acquire spectra (a) that should be aligned prior summing them (b). This is also referred to as energy channel calibration.

- The alignment is often manual - requires user feedback
- Almost always assumes linearity;
  - two coefficients **Energy** = $\alpha * $ **channels +** β

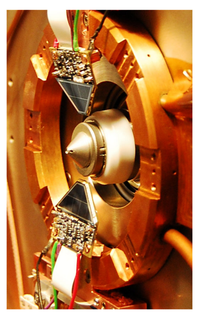




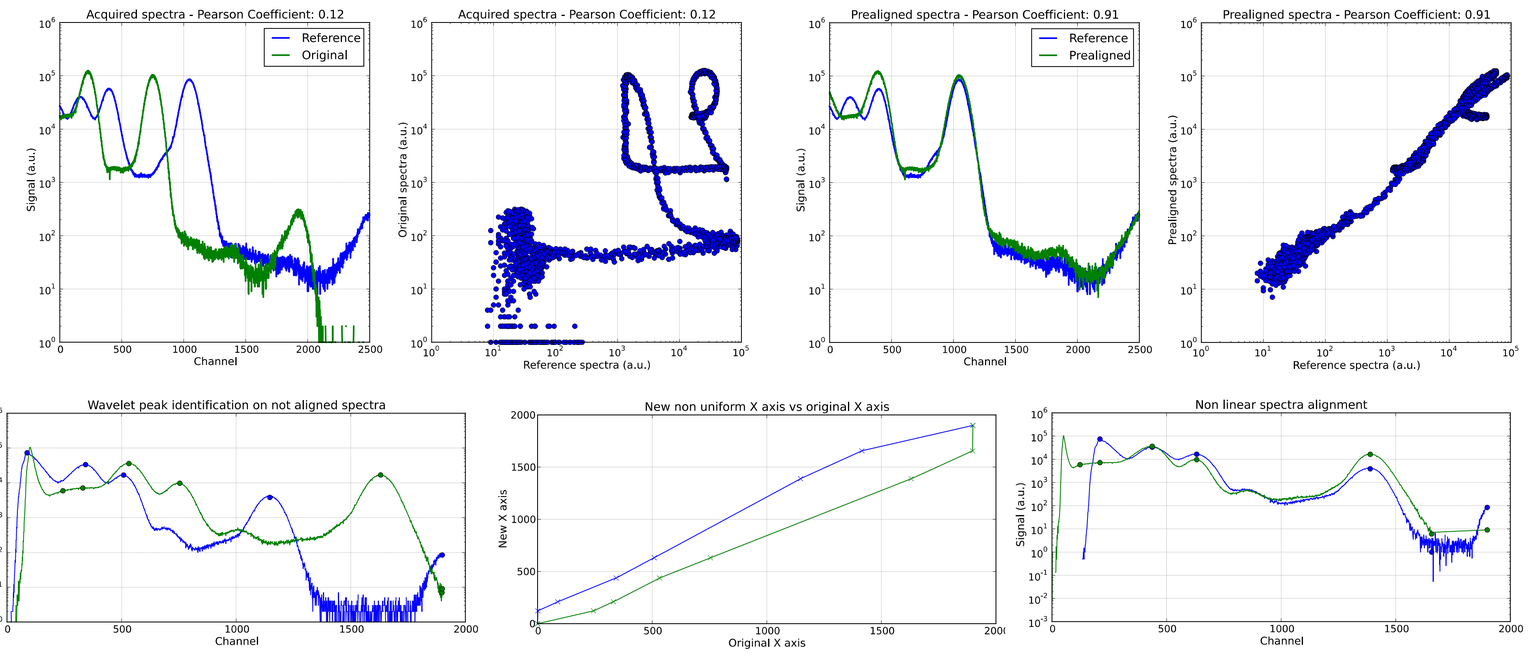
Proposed method [ref. 1]

1. Pre-alignment (linear)
   - as minimisation problem using a Pearson product-moment correlation between different detectors

2. Non-linear alignment (refinement)
   - peak identification (wavelets)
   - global interpolation function



- Automated, fast, efficient and more precise
- For multi-detector systems
- Specialised for XRF data (was compared to chromatographic profile [2] and NMR [3] methods)
- May make a difference in trace elements / low statistics studies
- In use at TwinMic beamline [4]:
  - 8 SDDs PNSensor, MCAs XGLab [5]
  - New multi-element Detector System [6]



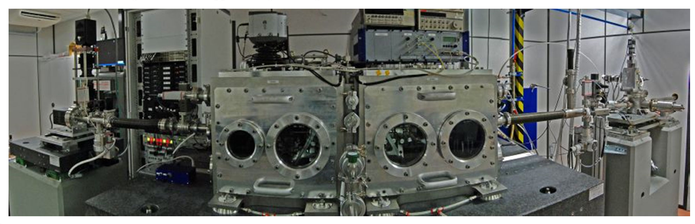
Introducing it to the workflow of a working Beamline is a challenge

Framework **DonkiOrchestra** [7]
- TANGO, ZeroMQ
- Scalable, Flexible, and Fast
- Concurrency & Workflow
- Publisher/Subscriber model
- Allows for extending acquisition systems already in operation.

Elements
- Director
- Players
- Triggers

Planning (Pre-Acquisition)	Collection (Data Acquisition)	Closeout (Post-Acquisition)
• **Players** Tango devices are defined in an XML • **Priorities** are read from the players (scalability) • **Pre-operation** signal sento to the players	• The **sequence of triggers** is sent to the players with a “**priority based**” partition • DAQ players push data with a **'trigger number'** tag • A pool of internal threads acquires and writes data to **HDF5 files**	• **Closeout-operation** signal is sent to the players

Beamline TwinMic [4]
- Imaging and Fluorescence
- **XRF**, STXM, Fullfield, CDI, Ptychography



Scanning
- LabView (in the past)
- DonkiOrchestra (in development)
- Trigger/Event-recording HDF5
- Alignment method in “**closeout Phase**”
- But also used as a guess during Collection

Tuesday 18th, 16:00
talk by Roberto Borghes !

[1] G. Kourousias, F. Billè, A. Gianoncelli. X-Ray Spectrometry (*in press*)
[2] JWH. Wong, G. Cagney, H. M. Cartwright, Bioinformatics 21(9),2005, 2088-2090.
[3] F. Savorani, G. Tomasi, SB Engelsen. Journal of Magnetic Resonance 202(2), 2010, 190-202.
[4] A. Gianoncelli, G. Kourousias, L. Merolle, M. Altissimo, and A. Bianco (2016). J. Synchrotron Rad. 23. and [https://www.elettra.eu/elettra-beamlines/twinmic.html]
[5] A. Gianoncelli, G. Kourousias, A. Stolfa, B. Kaulich Journal of Physics (A), Vol. 425 - 18, pp. 182001 (2013)
[6] A. Gianoncelli et al., Nuclear Instruments and Methods in Physics Research A vol. 816, 2016, pp. 113-118
[7] R. Borghes et al. **DonkiOrchestra**: *a scalable system for data collection and experiment management based on ZeroMQ distributed messaging*, NOBUGS 2016

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