A standard data format for XAS & XRF

Our (partial) wishlist

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DESY

Overview

> My personal perspective

> From our XRF-perspective:

- Current file-format issues
- Software issues

> From our XAS-perspective:

- Current file-format issues
- Software issues

> Our (partial) Wishlist

Personal perspective: P06 Hard X-Ray Micro/Nano-Probe

Our task: Provide **micro- and nanometer X-ray beams** from 2.4 – 100 keV to be used with a **multitude of different contrast mechanisms** **(**XRF, XRD, XAS, CDI, phase + absorption tomography, …)

Currently under commissioning …

Interested in changing our data format while this is still easy …

X-Ray Fluorescence (XRF)

Implications of the current file format (FIO)

- Current situation at beamline L: Pixel dwell times ~ s, single scan duration ~ hours
  - ➔ Several 10K ASCII-files per scan
  - ➔ Spectral fitting can be done on normal PCs (~ 2 spectra / second and core)
  - ➔ Each operation involves reading a FIO file, converting from ASCII, fitting, converting to ASCII, writing an ASR-file

- Estimate for P06 Microprobe: Dwell times ~ ms
  - ➔ Data evaluation in near-real-time requires much faster access to spectral data
  - ➔ Several million files per scan: File system + conversion is becoming a **severe bottleneck**

➔ **Quickly** progressing to a HDF5-based standard data format could be very helpful.

X-Ray Fluorescence (XRF) continued

Implications on the software / workflow:

- **AXIL / MICROXRF2:** Spectral fitting package, developed by Prof. Vincze's groups (Gent)
  - Primarily used at beamline L, will also be available at P06
  - Relies on single spectrum/file
  - Support for HDF5 is not clear
  - A lot of evaluation scripts written by users relies on FIO + ASR
- **PyMca:** Spectral fitting + visualization package, developed by A. Solé (ESRF)
  - Available at beamline L, P06 + P11
  - Can read FIO and HDF5
  - Open source (Python), package is still being extended (e.g. XAS, 3d-visualization etc.)
- **XRDUA:** Diffraction + fluorescence tomography package, developed by de Nolf (Antwerp)
  - Available at beamline L, P06 + P11
  - Open source (IDL), support will most probably continue by either Antwerp or ESRF

➔ Progression to an HDF5-based SDF will affect the workflow
(read: require work on the side of the beamline scientists),
but software solutions exist or software can be adapted

➔ Important for backward compatibility: **Converter from SDF to FIOs**

X-ray Absorption Spectroscopy (XAS)

Implications of the current fileformat (FIO)

> Current situation at the EXAFS-beamlines:

- One FIO per XAS-scan, takes ~ several minutes
- Full spectral data is typically recorded but almost never taken into account
- Evaluation of XAS-data is limited by the availability of experts and measured in PhD-weeks rather than in seconds

> Future estimate:

- QEXAFS: Time per spectrum ~ 0.1s ➔ Creation of FIO-files could start to become a problem
  (BMBF project R. Frahm)
- 100 element detector: n x 100 columns FIO files could push evaluation software to and beyond their limits
  (BMBF project G. Henkel + W. Meyer-Klaucke)

➔ The XAS-community ***could*** continue to use FIO-files

➔ but in the near future, the FIO-fileformat will also become a handicap

➔ PETRA III extension might be the ideal opportunity to progress to the SDF.

X-ray Absorption Spectroscopy (XAS) continued

Implications on the software / workflow:

- **Feff/Athena/Artemis etc.:** Standard XAS evaluation package, developed by J. Rehr, B. Ravel & M. Newville & Co (US)
- **WinXAS:** Developed by T. Ressler
- **Viper:** Developed by K. Klementiev (ALBA)
- **DL_EXCURV / ABRA / KEMP:** BioXAS software, developed by CCP3 / W. Meyer-Klaucke + G. Wellenreuther
  - Can all use FIO-files
  - HDF5-support is not yet available, but is being discussed

➔ The XAS-community will be able to benefit from the SDF **if** the standard software packages adopt it

➔ Again: Important for backward compatibility: **Converter from SDF to FIOs**

➔ SDF should support use of the **full spectral data** for better / easier EXAFS-extraction / post-processing

Our (partial) Wishlist

- XRF: **Get SDF** implemented as an option **as soon as possible.**
- XRF: **Coordinate efforts with ESRF / A. Solé** in order to have software supporting XRF+SDF from day 1.
- XAS: Coordinate efforts with e.g. **M. Newville / K. Klementiev / R. Frahm / G. Henkel** to have software supporting XAS+SDF as soon as possible.
- XRF + XAS: Ensure support for **mixed methods** in SDF.
- XRF + XAS: Ensure **availability of tools** for SDF **from day 1**, especially
  - An **SDF-to-ASCII** creator (to create generic Comma-Seperated-Values files including selected header information)
  - An **FIO-extractor** (result should be as close to FIO as possible).