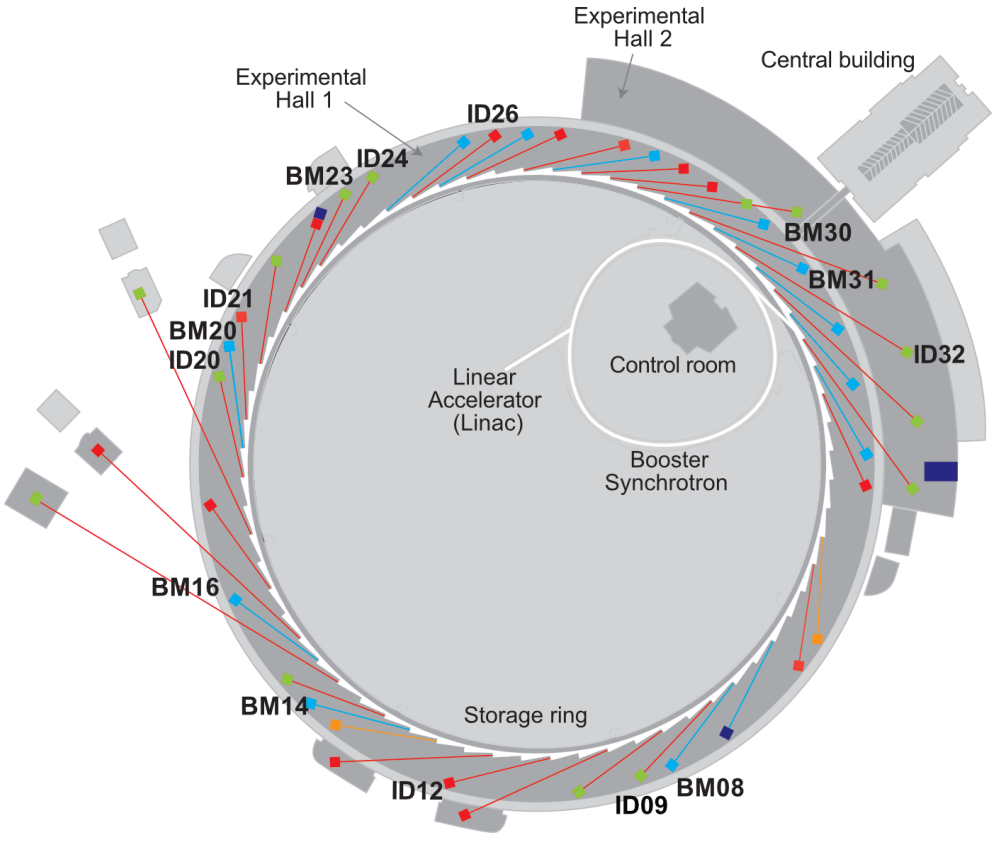
Overview of data analysis tools and computational software

Marius Retegan
Algorithms & Scientific Data Analysis Group
Experiments Division

SPECTROSCOPY BEAMLINES AT ESRF



	XAS	XMCD	XES	RIXS
ID09			✓	
ID12	✓	✓		
ID20	✓	✓	✓	✓
ID21	✓			
ID24	✓		✓	
ID26	✓	✓	✓	✓
ID32	✓	✓		✓
BM08	✓			
BM14	✓			
BM16	✓		✓	✓
BM20	✓		✓	✓
BM23	✓			
BM30	✓			
BM31	✓			

XAS – X-ray Absorption, **XMCD** – X-ray Magnetic Circular Dichroism
XES – X-ray Emission, **RIXS** – Resonant Inelastic X-ray Scattering

DATA REDUCTION AND ANALYSIS FOR SPECTROSCOPY

1. Getting from raw data to publishable plot

    - spectra averaging, rebinning, etc.
    - background subtraction
    - outliers removal
    - plotting

2. Interpreting and understanding the experimental data

    - assignment of spectral features
    - extraction of structural and electronic properties: oxidation state, bond lengths, crystal field parameters, etc.

ESRF-EBS: A NEW CONTROL SYSTEM AND DATA FORMAT

Beam**L**ine **I**nstrumentation **S**upport **S**oftware

The BLISS control system provides a global approach to running synchrotron experiments requiring synchronously controlled motors, detectors, and various acquisition devices thanks to hardware integration, Python sequences, and an advanced scanning engine.

HDF5 is file format to organize large amounts of data.

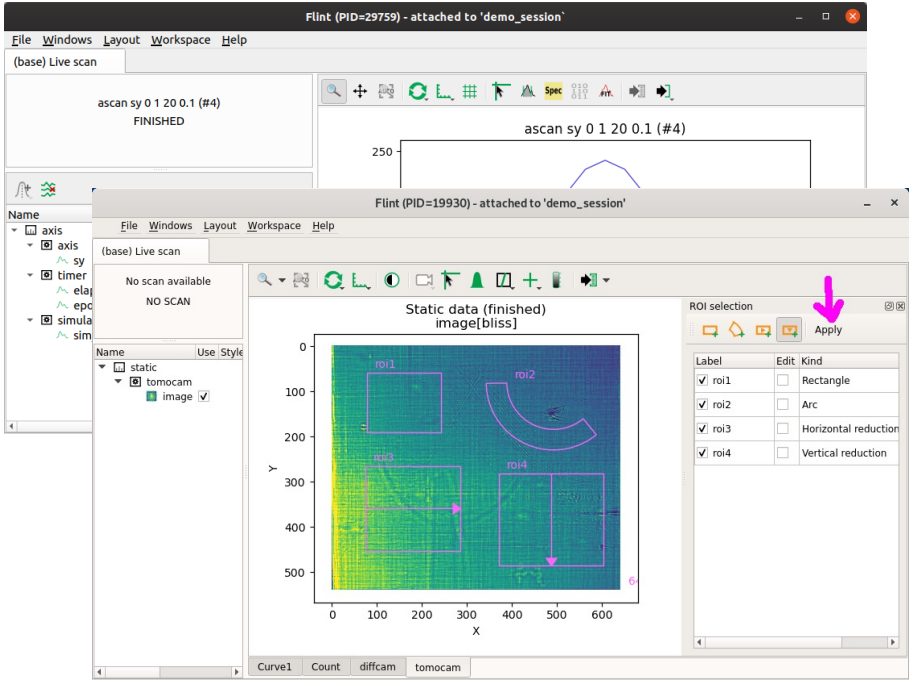
NeXus

Adds additional rules and structure to help people and software understand how to read a HDF5 file.

https://manual.nexusformat.org/impatient

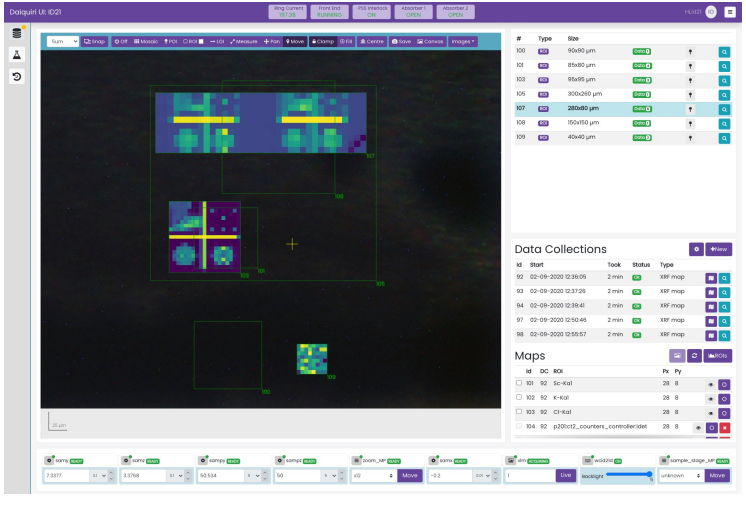
TOOLS TO VISUALIZE AND ANALYZE EXPERIMENTAL DATA

Flint is the GUI companion for BLISS that provides a live display for current scans.



Daiquiri is a Python-based framework for beamline control and data acquisition.

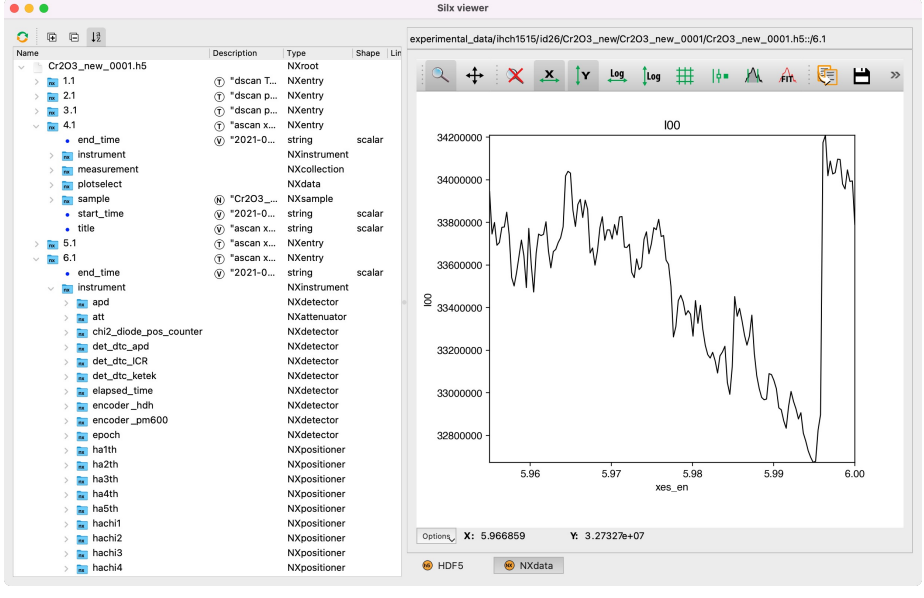
Daiquiri UI is the web-based JavaScript User Interface for Daiquiri.



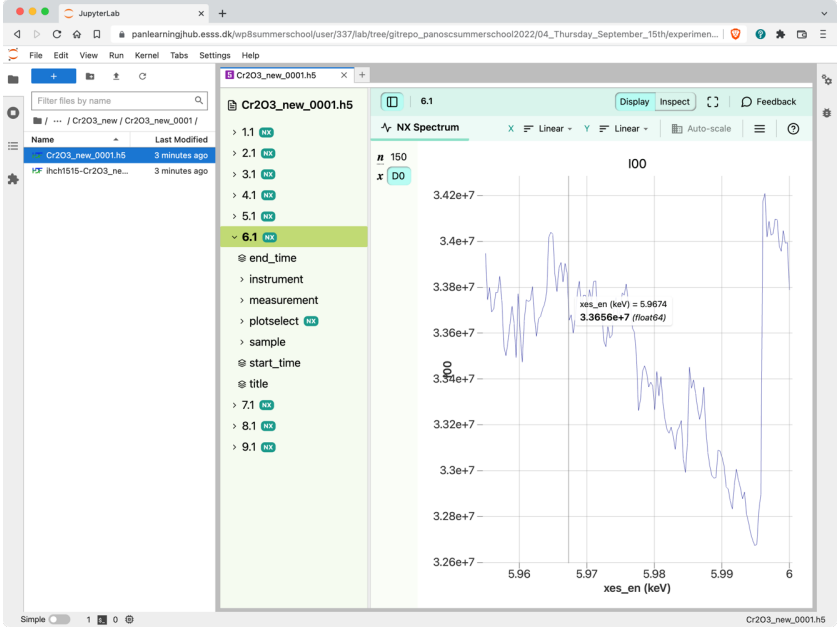
https://bliss.gitlab-pages.esrf.fr

TOOLS TO VISUALIZE AND ANALYZE EXPERIMENTAL DATA

silx view a unified viewer for HDF5, SPEC, and image file formats



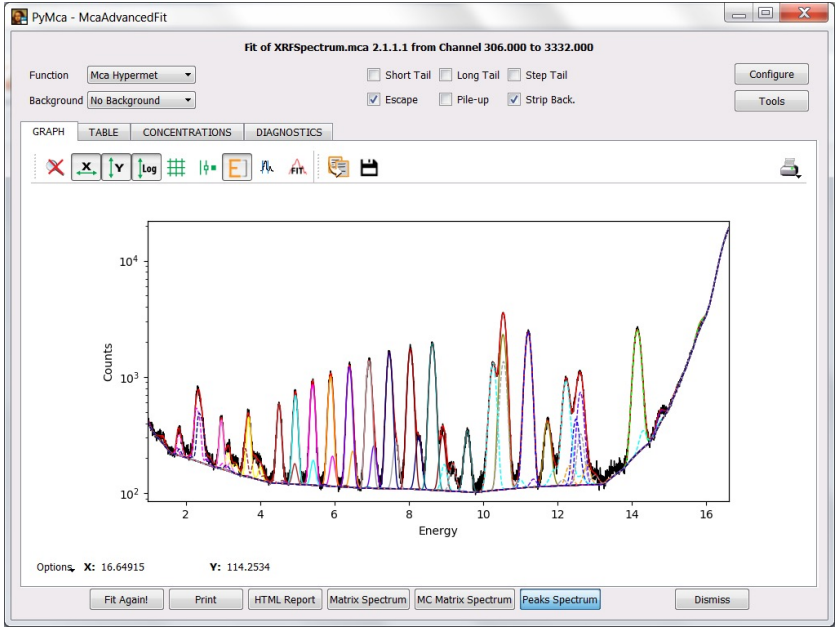
h5web a collection of components to visualize and explore data

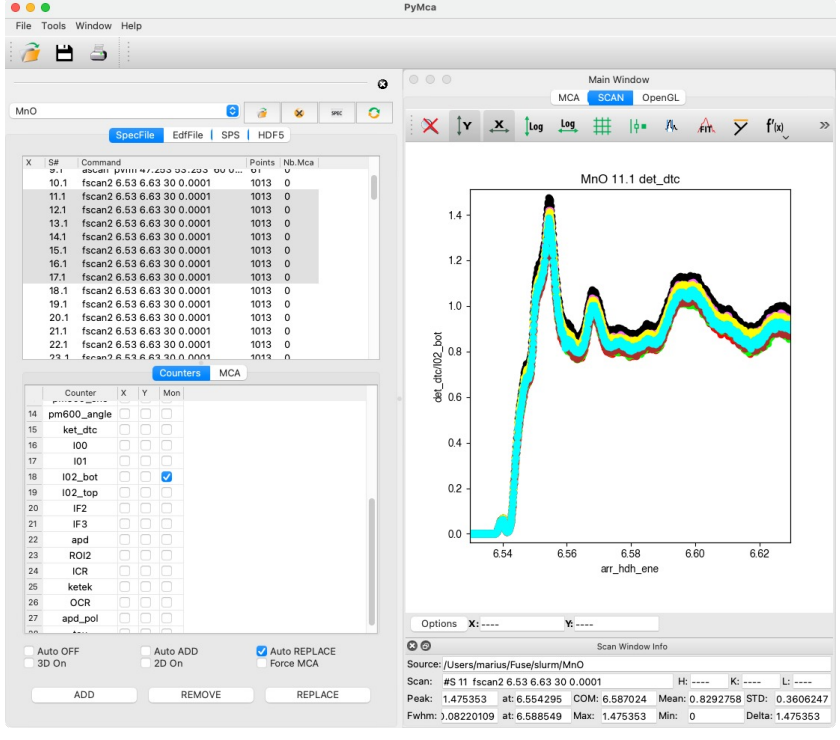


http://www.silx.org

TOOLS TO VISUALIZE AND ANALYZE EXPERIMENTAL DATA

PyMCA is a ready to use, and in many aspects state-of-the-art, set of applications implementing most of the needs of X-ray fluorescence (XRF) data analysis.





http://www.silx.org

TOOLS TO VISUALIZE AND ANALYZE EXPERIMENTAL DATA

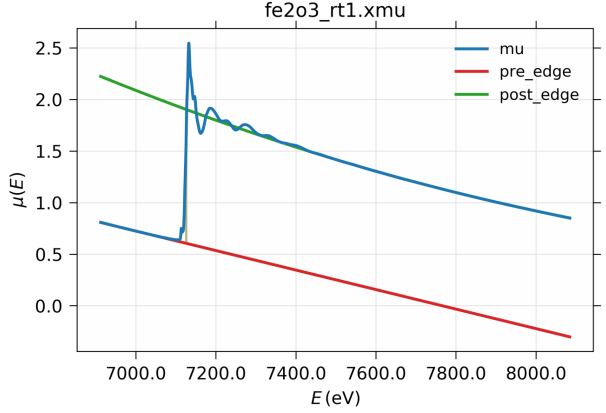
Larch is an open-source library and set of applications for processing and analyzing X-ray fluorescence (XRF) and X-ray absorption spectroscopy (XAS).

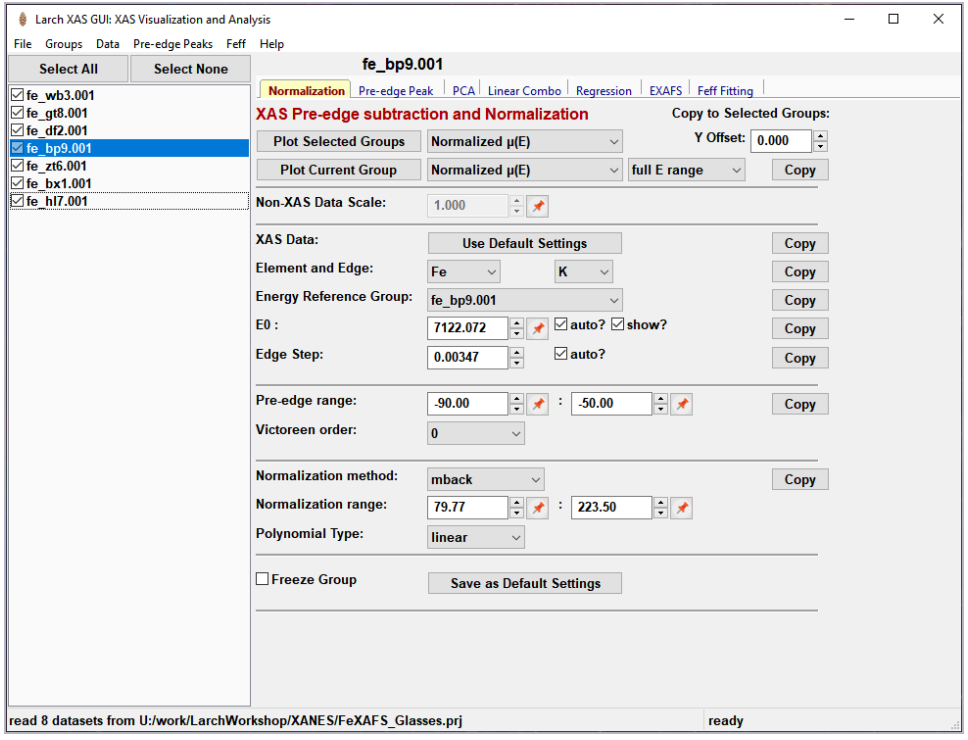
```
from larch.io import read_ascii
from larch.xafs import pre_edge
from wxmplot.interactive import plot

fname = 'fe2o3_rt1.xmu'
dat = read_ascii(fname, labels='energy mu i0')

pre_edge(dat, group=dat)

plot(dat.energy, dat.mu, label='mu', xlabel='Energy (eV)',
     title=fname,show_legend=True)
plot(dat.energy, dat.pre_edge, label='pre-edge line')
plot(dat.energy, dat.post_edge, label='post-edge curve')
```





https://millenia.cars.aps.anl.gov/xraylarch

TOOLS TO VISUALIZE AND ANALYZE EXPERIMENTAL DATA

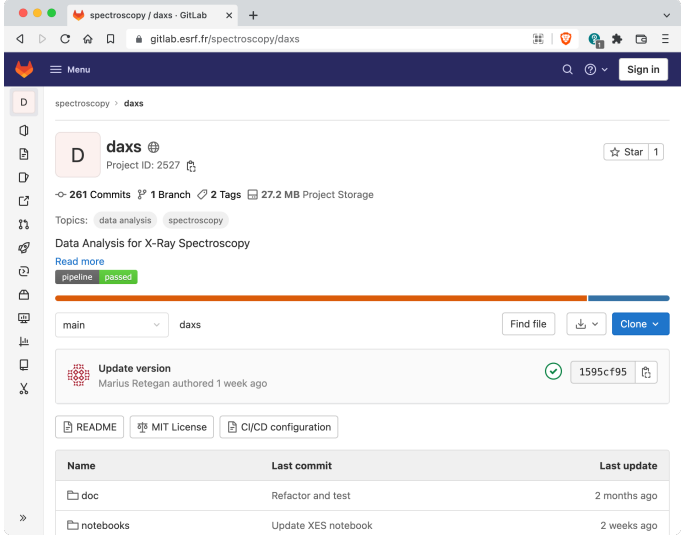
Visualization

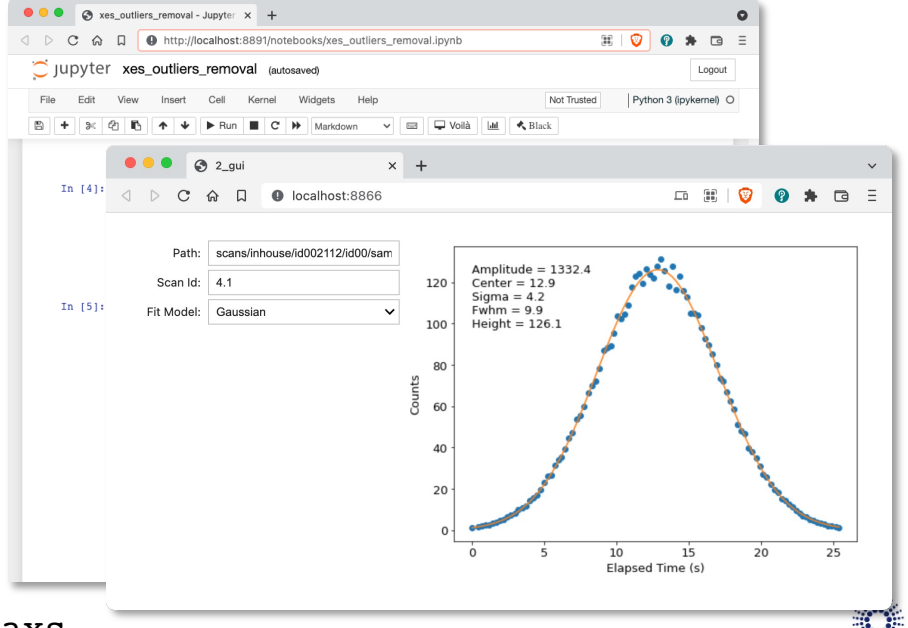
Several tools can be used to look at the acquired data during an experiment: **Flint, Daiquri, silx view, h5web**

Analysis

There are a plethora of tools to analyze XANES/EXAFS data: **PyMCA, Larch, GNXAS, PyFitIt**

The analysis tools are focused on XAS, and there are no tools to treat XES or RIXS measurements.

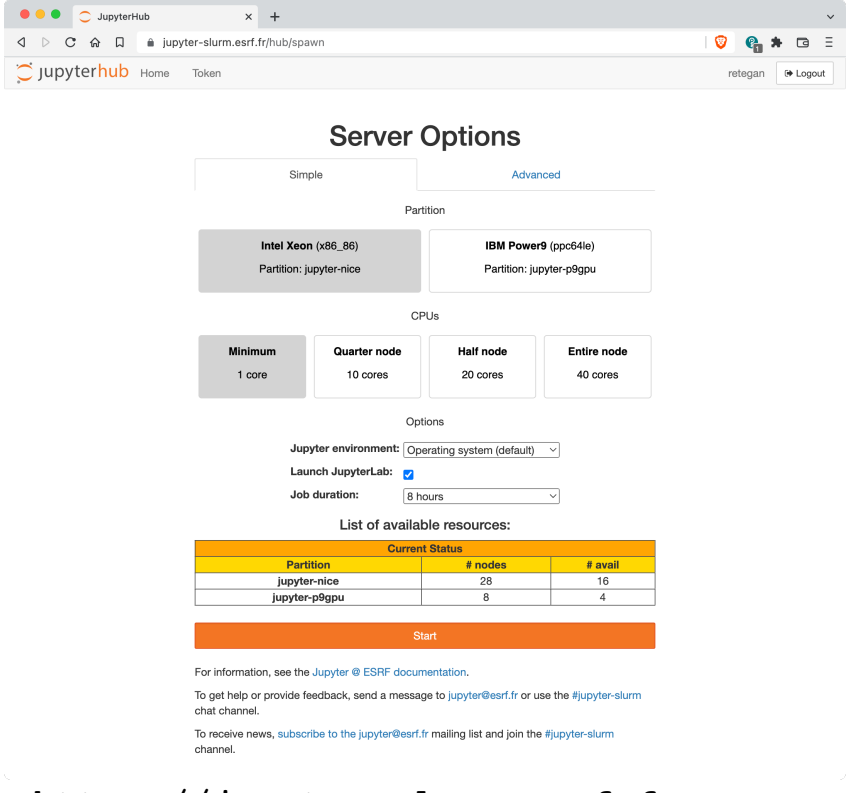


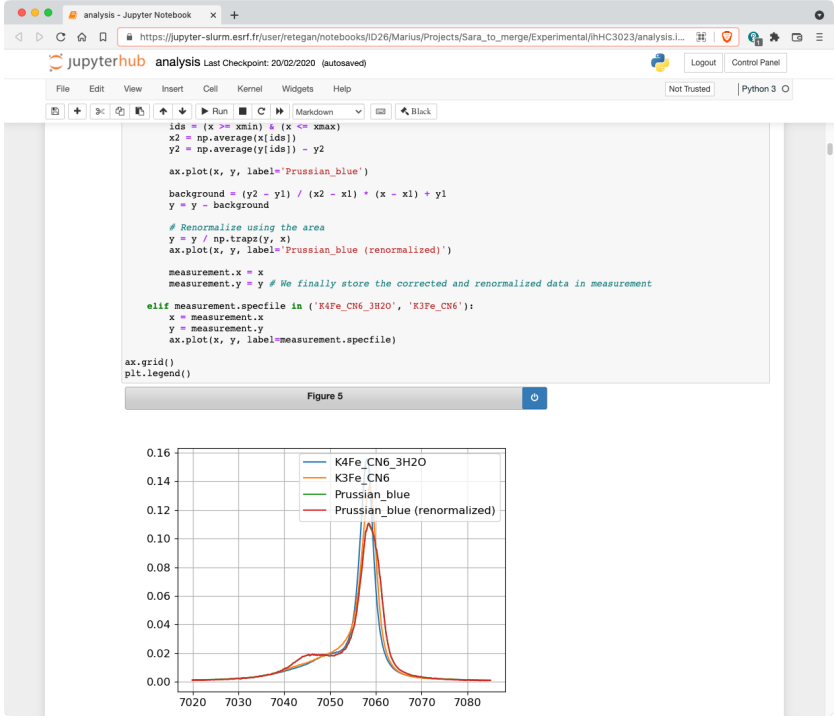


https://gitlab.esrf.fr/spectroscopy/daxs

JUPYTERHUB AT ESRF

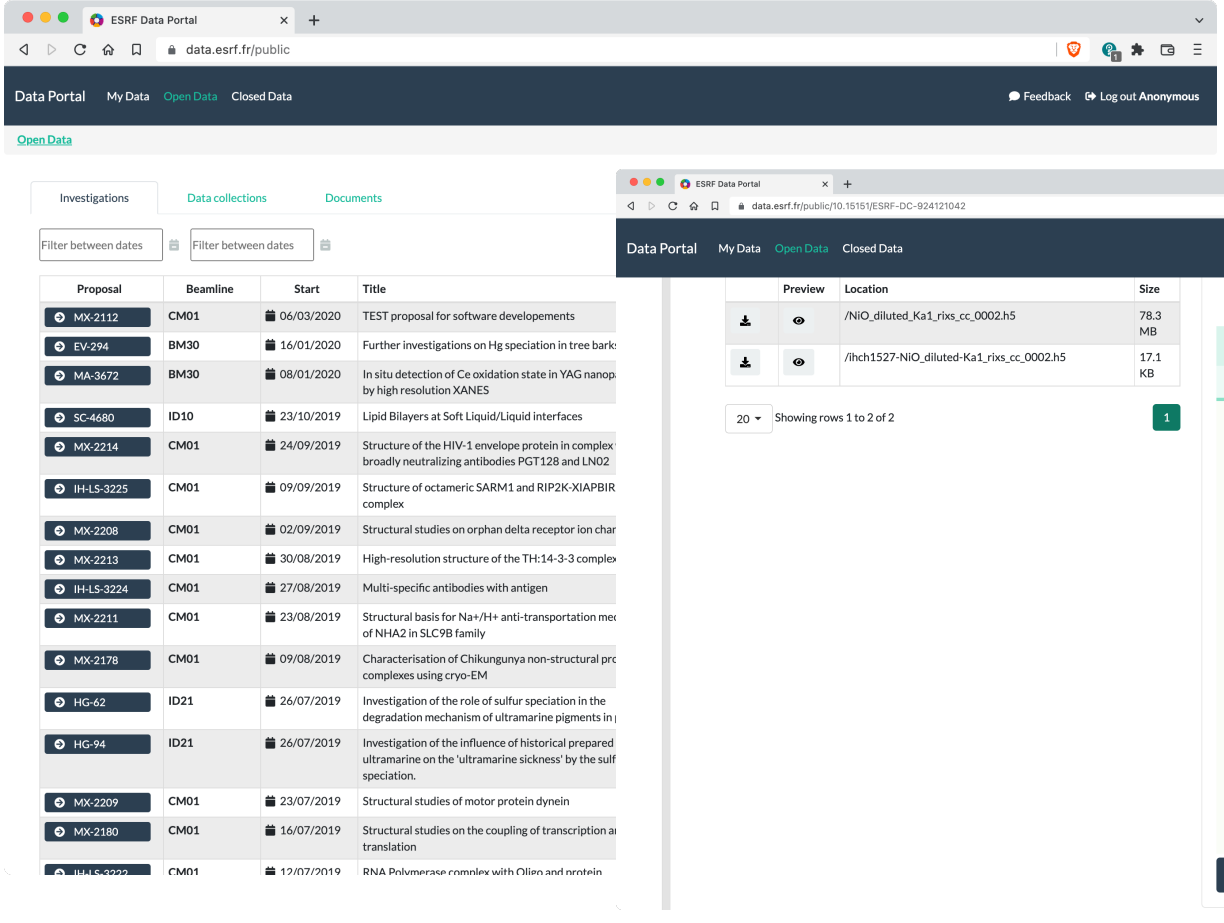
The JupyterHub installation can be used to access computing resources and measured data.





https://jupyter-slurm.esrf.fr

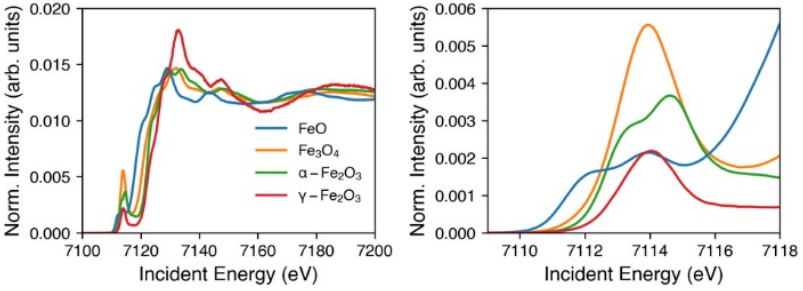
THE ESRF DATA CATALOGUE



https://data.esrf.fr

X-RAY SPECTROSCOPY: EXPERIMENT AND COMPUTATION

Experimental X-ray spectroscopy data are often evaluated by comparison to reference compounds.



Computational X-ray spectroscopy provides a deeper insight by ***maximizing*** the amount of information that can be extracted from the experimental data.

Specialized *ab initio* codes:

FEFF, FDMNES, OCEAN, …

Generic *ab initio* codes:

ORCA, MOLCAS, ADF, Wien2k, VASP, Quantum ESPRESSO, …

Semi-empirical multiplets codes:

Cowan's Codes (RCN), Quanty, Xclaim, XTLS, Hilbert++, …

SEMI-EMPIRICAL MULTIPLETS: THE EARLY DAYS

atoms

MDPI

Article

Cowan Code: 50 Years of Growing Impact on Atomic Physics

Alexander Kramida

National Institute of Standards and Technology, Gaithersburg, MD 20899, USA; alexander.kramida@nist.gov

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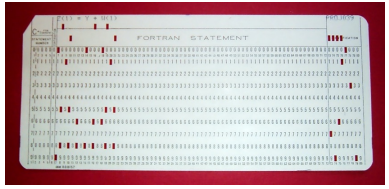
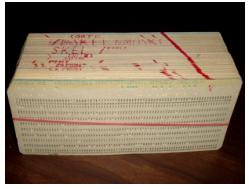
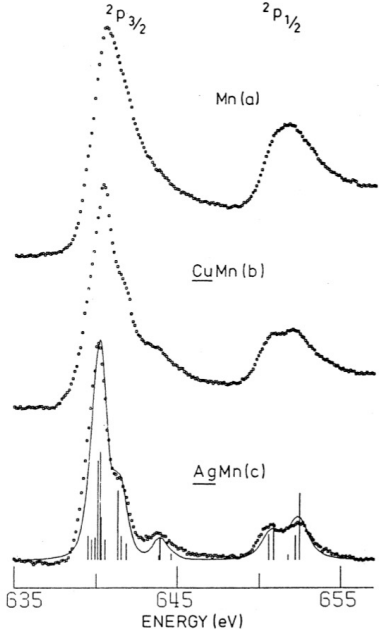
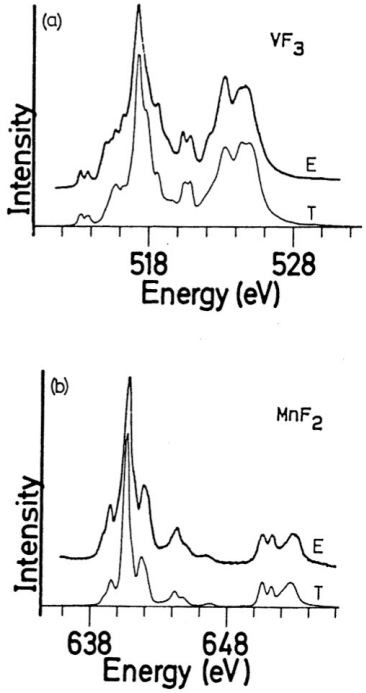
check for updates





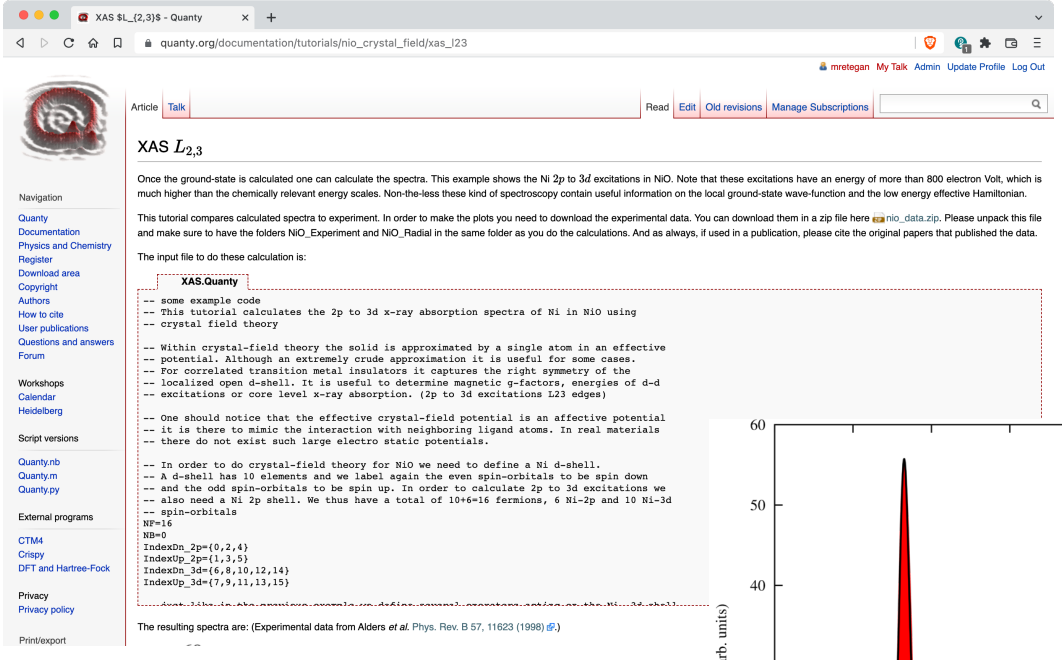


B.T. Thole *et al.*,
Phys. Rev. B, 31, **1985**



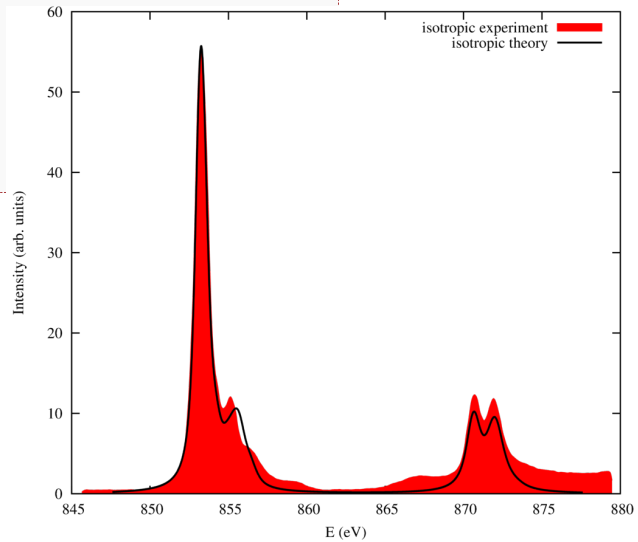
F.M.F. de Groot *et al.*,
Phys. Rev. B, **1990**

QUANTY: A MODERN APPROACH TO MULTIPLETS CALCULATIONS



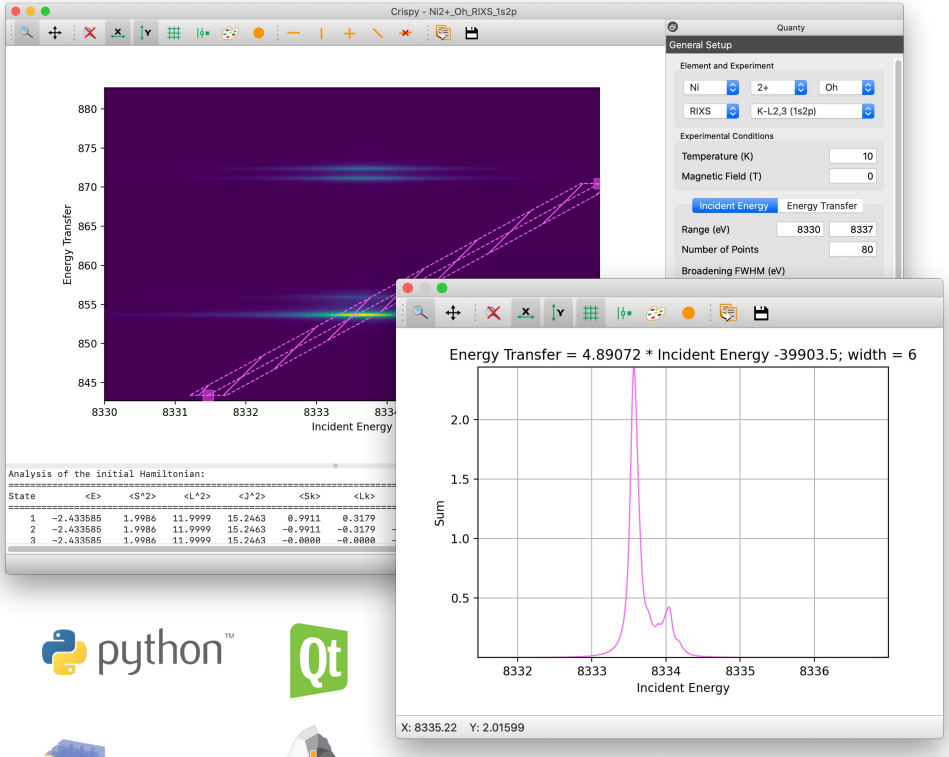
Quanty is a powerful and versatile library, but…

- You will have to write code to perform calculations.
- The program is very forgiving, and it can take a long time to spot an error.



https://quanty.org

CRISPY: A GRAPHICAL USER INTERFACE FOR MULTIPLETS CALCULATIONS



Calculations:

- transition metals, lanthanides, and actinides
- XAS, XMCD, X(M)LD, XES, XPS, and RIXS
- a large number of edges
- O_h, D_{4h}, C_{3v}, T_d, and D_{3h} symmetries

Additional features:

- logging console to display the progress
- dialog showing the details of a calculation
- interactive broadening using FFT
- save and load functionality
- easy-to-use installers for Windows and macOS
- Jupyter notebook interface

https://github.com/mretegan/crispy

SEMI-EMPIRICAL MULTIPLETS: THE HAMILTONIAN

$$H = \underbrace{H_{kin} + H_{en} + H_{ee} + H_{so}}_{\text{Free ion (spherical)}} + \underbrace{H_{cf}}_{\text{Crystal Field}} + \underbrace{H_{hyb}}_{\text{Hybridization}} + \underbrace{H_{Zeeman}}_{\text{Magnetic Field}} + \underbrace{H_{ex}}_{\text{Exchange}}$$

$$H_{kin} = -\sum_i \frac{\hbar^2 \nabla_i^2}{2m}$$ Kinetic energy of the electrons

$$H_{en} = -\sum_i \sum_I \frac{Z_I e^2}{|r_i - R_I|}$$ Electron–nuclear interaction

$$H_{ee} = \frac{1}{2} \sum_i \sum_{j \neq i} \frac{e^2}{|r_i - r_j|}$$ Electron–electron interaction

$$H_{so} = \sum_i \xi(r_i) l_i \cdot s_i$$ Spin–orbit interaction

$$H_{cf} = \sum_{k=0}^{\infty} \sum_{m=-k}^{k} r^k A_{k,m} C_{k,m}(\theta, \phi)$$ Crystal field potential

SEMI-EMPIRICAL MULTIPLETS: THE PARAMETRIZATION PROBLEM

Electronic repulsions: direct and exchange integrals

The Slater radial integrals are reduced from their Hartree–Fock values using empirical reduction factors.

$0.7 \leq \kappa \leq 0.9$ ionic character

$0.5 \leq \kappa \leq 0.6$ covalent character

Spin-orbit coupling constants

They are usually close to the Hartree–Fock atomic values.

Crystal field parameters

Initial values are usually taken from other spectroscopies or calculations

10Dq for octahedral symmetry (O_h)
Dq, Ds, Dt with a tetragonal distortion (D_{4h})

Hybridization (configuration interaction) parameters

Many ad hoc parameters: $\Delta, U_{dd}, U_{pd}, V(e_g), V(t_{2g})$