

ESRF + PaNdata

Update on activities

Summary

- Software catalog
- Data Policy
- Metadata
- Silx library
- Calypso+
- XSOCS
- Jobs



Software Catalog – thanks Jamie (ILL) !

PaNdata Softwa... x +

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PaNdata Software Catalogue


PaNdata software catalogue is a database of software used mainly for data analysis of neutron and photon experiments.


This database can be freely consulted. It gives an overview of software available for neutron and photon experiments and their use with respect to instruments at experimental facilities.


By [registering](#) and [logging-in](#) new software can be entered and it will appear in the database after moderation.

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Recently added software


 **ANKAphase**
ANKAphase processes X-ray inline phase-contrast radiographs by reconstructing the projected thickness of the object(s) imaged. The tool uses a single-...


 **BONSU**
Bonsu is an interactive phase retrieval suite, designed for phase retrieval with real-time visualisation in both two and three dimensions. It includes...




Map of Europe showing experimental facilities: ESS, HZB, MAX IV, diamond, ISIS, LEIL, PSI, ESRF, and others.

Recently updated software

 **iFit**

 **ANKAphase**

 **WIEN2k**

Software Catalog — thanks Claudio (ESRF) !


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 **ABINIT**

ABINIT is a suite of programs for materials science, which implements density functional theory, using a plane wave basis set and pseudopotentials, to compute the electronic density and derived properties of materials ranging from molecules to surfaces to solids. It implements density functional theory by solving the Kohn–Sham equations describing the electrons in a material, expanded in a plane wave basis set and using a self-consistent conjugate gradient method to determine the energy minimum. Computational efficiency is achieved through the use of fast Fourier transforms, and pseudopotentials to describe core electrons. As an alternative to standard norm-conserving pseudopotentials, the projector augmented-wave method may be used. In addition to total energy, forces and stresses are also calculated so that geometry optimizations and ab initio molecular dynamics may be carried out. Materials that can be treated by ABINIT include insulators, metals, and magnetically ordered systems including Mott-Hubbard insulators.

 **ANKAphase**

ANKAphase processes X-ray inline phase-contrast radiographs by reconstructing

Data Policy

—

implementation

status



Beamline	Status	Techniques	Metadata Collection*	Data archiving*	Raw Data HDF5*	Open access to data*
ID01		KMAP	implemented			
BM01A						
BM01B						
ID02						
BM02						
ID03						
BM05		Tomography	In progress			
ID06-LVP						
ID06		Tomography	In progress			
BM08						
ID09						
ID10						
ID11		Tomography	In progress			
ID12						
ID13						
BM14						
BM15A						
BM15B						
ID16A-NI		Fluo, Tomo	implemented		implemented	
ID16B-NA		Fluo,Tomo	In progress			
ID17		MRT, Tomography	implemented			
ID18						
ID19		Tomography	In progress			
ID20						
ID21		Diffraction	In progress			
ID22						
ID23-1		MX	In progress			
ID23-2						
BM23						
ID24						
BM25A						
BM25B						
ID26			In progress			
BM26A						
BM26B						
ID27						
ID28						
BM28						
ID29		MX	implemented			
BM29		BIOSAXS	implemented			
ID30A-1		MX	implemented			
ID30A-3		MX	implemented		implemented	
ID30B		MX	implemented			
BM30A						
BM30B						
ID31						
ID32			In progress			
BM32						

Rich Metadata in ICAT + HDF5

(following Nexus conventions)

- technique_name
- InstrumentSource_mode
- InstrumentSource_current
- InstrumentInsertionDevice_gap_value
- InstrumentInsertionDevice_taper_value
- Sample_description
- InstrumentMonochromator_wavelength
- InstrumentMonochromatorCrystal_usage
- InstrumentMonochromatorCrystal_d_spacing
- InstrumentMonochromatorCrystal_type
- InstrumentMonochromatorCrystal_reflection
- InstrumentSlitPrimary_vertical_gap
- InstrumentSlitPrimary_vertical_offset
- InstrumentSlitPrimary_horizontal_gap
- InstrumentSlitPrimary_horizontal_offset
- InstrumentSlitPrimary_blade_up
- InstrumentSlitPrimary_blade_down
- InstrumentSlitPrimary_blade_front
- InstrumentSlitPrimary_blade_back
- InstrumentSlitSecondary_vertical_gap
- InstrumentSlitSecondary_vertical_offset
- InstrumentSlitSecondary_horizontal_gap
- InstrumentSlitSecondary_horizontal_offset
- InstrumentSlitSecondary_blade_up
- InstrumentSlitSecondary_blade_down
- InstrumentSlitSecondary_blade_front
- InstrumentSlitSecondary_blade_back
- InstrumentSlits_vertical_gap

Silx library

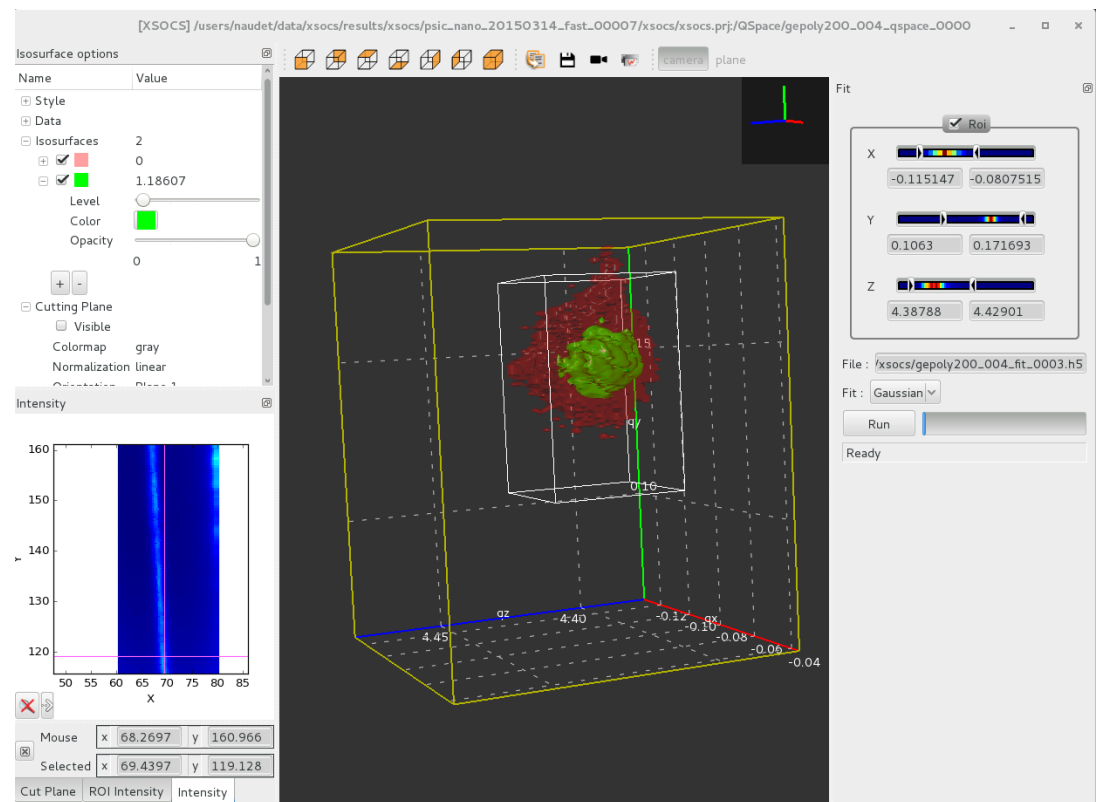
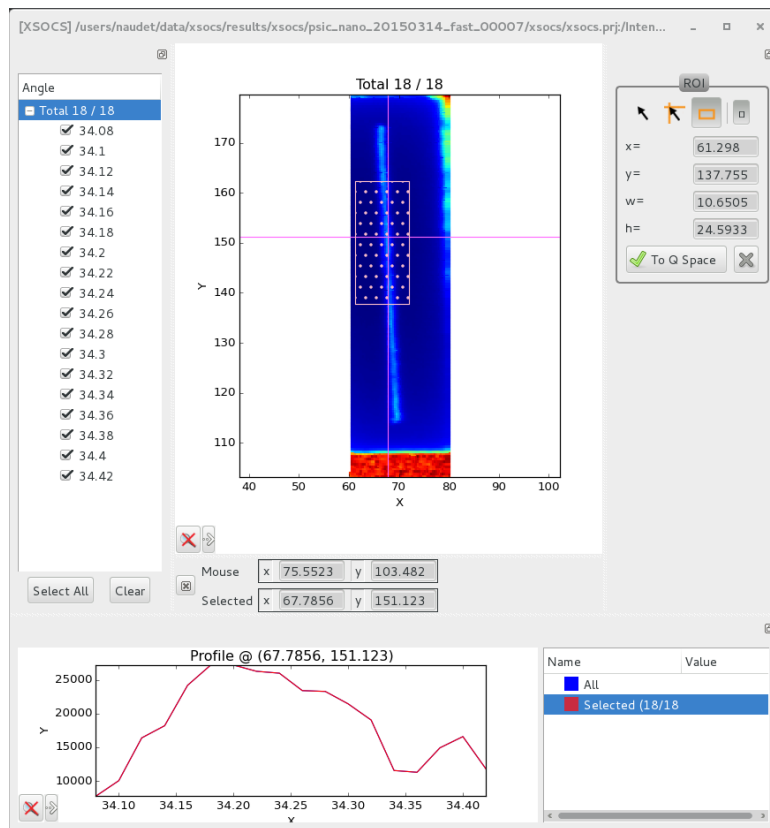
- Python Library to serve as platform for scientific applications for photon science
- Planned to invest 20 years FTE, 5 invested since 2016
- Main library : <https://pythonhosted.org/silx/>
- Fourth release 0.4.0 includes HDF5 + 3D support
- More and more applications building on silx e.g. XSOCS, Scarpy, PyFai, PyMca, Fabio, ...
- Checkout : <https://github.com/silx-kit/silx>
- Slides from training held at ALBA last month :
<https://cloud.esrf.fr/index.php/s/c3QwF9meYlOA8KB>

Other projects

- NFFA – metadata + data analysis (XSOCS)
- Calypsoplus – kickoff May 2017
- NeXT – submitted to EINFRA-21
- PaNDaaS – resubmission in 2018 (?)
- LEAPS – IT work package for Photon Sources for the next N years

XSOCS – nanostrain scanning

- Example of improving existing scientific software by **orders of magnitude** ...



Job – ESRF is looking for Data Manager #2

Feedback

Software Engineer for Data Management

Job Location: Grenoble, France
Job Title / Reference: Software Engineer for Data Management / Ref. COD/DMG
Post details: 3 Years Maximum
Salary: 32-40 k€ and additional allowances may apply
Application deadline: Tuesday, April 25, 2017
Application Details / Contact:
The ESRF, the European Synchrotron, is an international science facility based in Grenoble, France. Thanks to its high-level, innovative engineering and cutting-edge vision, the ESRF is recognised as one of the top research institutions worldwide, welcoming more than 6 500 scientists every year in fields such as biology, medicine, chemistry, earth and environmental sciences, cultural heritage, materials and surface science, and physics. The ESRF is supported by 21 countries and employs 600 staff.

[Apply online.](#)

Link to full posting: <http://www.esrf.eu/home/Jobs/engineering-rd-and-technical-opportunities.html>
Description:
In a team of 35 engineers and technicians, you will participate in a project focussing on the improvement of data management practices at the ESRF. In the context of the ESRF upgrade programme, the production of scientific data will evolve significantly both in complexity and in volume implying a significant change in the way data is

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Events

Proposal Deadlines

April 10, 2017
[Application Deadline: NXS 2017: 19th National School on Neutron and X-ray Scattering](#)

April 12, 2017
[1st Virtual LCLS User Meeting](#)

April 23, 2017
[Helmholtz-Zentrum Berlin : Young Investigators Workshop 2017](#)

May 1, 2017
[Tampa : Call for Abstracts](#)

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