

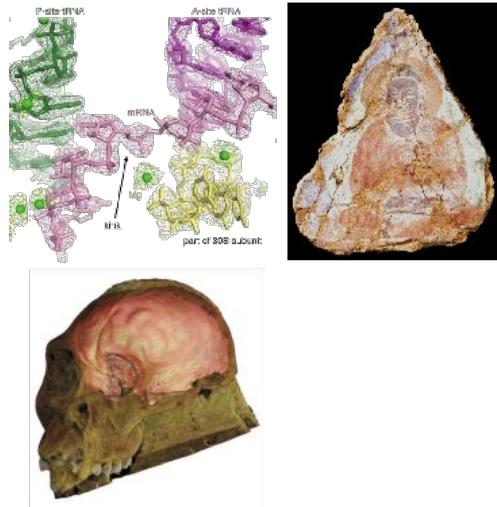
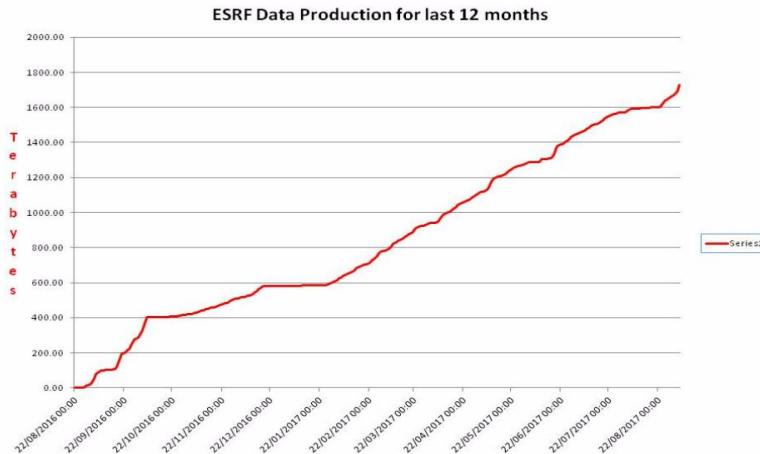
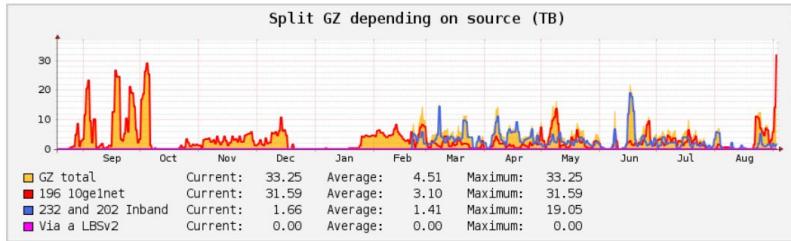
Data Management

@ESRF

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Software Engineer
Data Manager@Data Analysis Unit
Software Group
ESRF
Triestre 12/09/2018

Why a data management plan?

- Data is the raw material of science and is our main product



Why an ESRF data Policy?

Data needs to be properly managed to allow:

- Linking to publications (increasingly requested by publishers)
- Reanalyse
- Verification
- New research
- Preservation of unique data sets



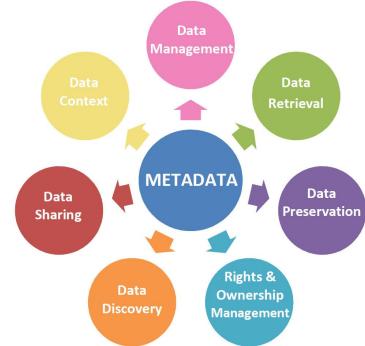
Data's shameful neglect

"Research cannot flourish if data are not preserved and made accessible. All concerned must act accordingly"

Nature 461, 145 (10 September 2009) | doi:10.1038/461145a

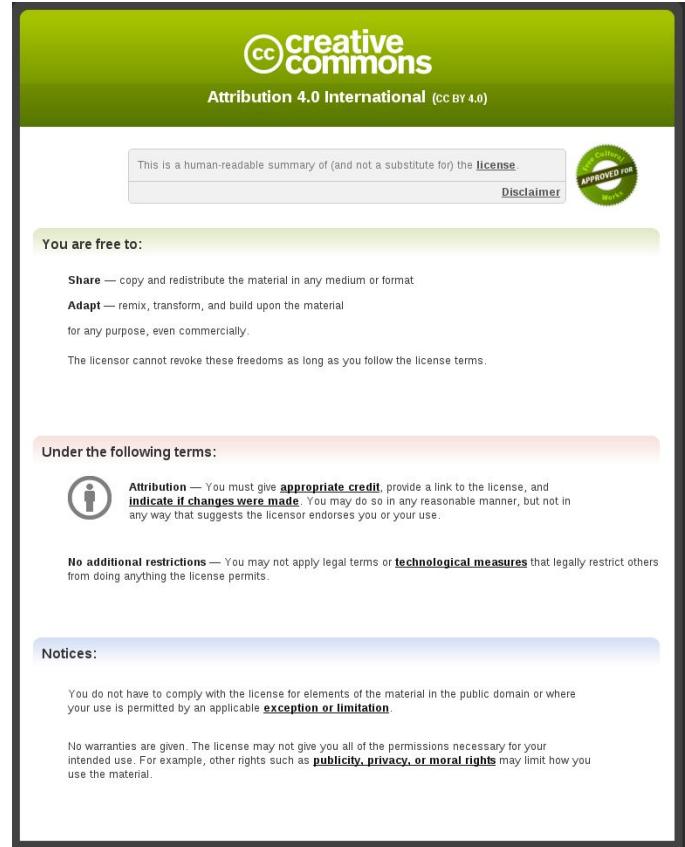
Data Policy General Principles

- **Automatic capture** of data and metadata
- ESRF is the keeper (**custodian**) of the raw data and associated metadata
- Raw data and metadata will be selected, organized and look after in **well-defined formats** (curation)
- Raw data and metadata will be **READ-ONLY** for the duration of their life time
- **Proprietary research** (commercial) will be owned exclusively by the client who purchased the access and it is not covered by the data policy
- Restricted to the experimental team during the **a period of 3 years** (EMBARGO)
- Access to raw data and associated metadata is foreseen to be via a **searchable online catalogue (ICAT)**



Data Policy

- About data and metadata
 - Only keep data generated at the ESRF
 - Data must be in a known format by the ESRF
 - Data must be traceable and verifiable as coming from the ESRF
- After the embargo the data will be released under the license CC-By-4



The image shows a screenshot of the Creative Commons Attribution 4.0 International license page. At the top, the Creative Commons logo is displayed next to the text "Attribution 4.0 International (CC BY 4.0)". Below this, there is a green banner with the text "This is a human-readable summary of (and not a substitute for) the [license](#)". To the right of this banner are links for "Disclaimer" and "Creative Commons License".

Under the banner, a section titled "You are free to:" contains two items: "Share" (copy and redistribute the material in any medium or format) and "Adapt" (remix, transform, and build upon the material). Both items are preceded by a brief description and a note that the licensor cannot revoke these freedoms as long as you follow the license terms.

Below this, a section titled "Under the following terms:" includes two items: "Attribution" (requiring credit to the original author) and "No additional restrictions" (prohibiting legal terms or technological measures that restrict use). Each item has a small icon next to it.

At the bottom, a section titled "Notices:" contains two paragraphs of fine print about the license's scope and limitations.

Benefits of Data Management



Fair Principles

Benefits of Data Management

What is FAIR DATA?



Data and supplementary materials have sufficiently rich metadata and a unique and persistent identifier.

FINDABLE



Metadata and data are understandable to humans and machines. Data is deposited in a trusted repository.

ACCESSIBLE



Metadata use a formal, accessible, shared, and broadly applicable language for knowledge representation.

INTEROPERABLE



Data and collections have a clear usage licenses and provide accurate information on provenance.

REUSABLE

Benefits of Data Management



What is FAIR DATA?



Data and supplementary materials have sufficiently rich metadata and a unique and persistent identifier.

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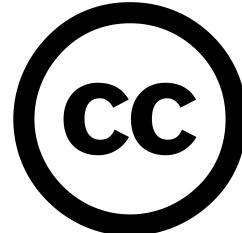
INTEROPERABLE



Data and collections have a clear usage licenses and provide accurate information on provenance.

REUSABLE

Nexus



**LOVE IT. HATE IT.
JUST DON'T FORGET TO USE IT.**



All our users agree to comply with the ESRF publication and data policy.
This includes correctly citing the DOI reference when publishing results based on ESRF data.

More info on <https://doi.esrf.fr>

Session

Dataset **Restricted access**PROTEINS AND PROTEIN/DNA/RNA COMPLEXES INVOLVED IN BIOSYNTHESIS, PROTEIN FOLDING AND DEGRADATION, SPLICING, CANCER,
HOST PATHOGEN INTERACTI

Roman FEDOROV ; Dominik MACHTENS ; Theresia REINDL ; Johannes CRAMER ; Patrick REINKE.

DOI

DOI 10.15151/ESRF-ES-115451959

Licence (for files)

Creative Commons Attribution 4.0

Proposal
MX-2080Publication year
2018Beamline
id30a3Session date
2018-8-28Category
Macromolecular Crystallography

Abstract

There is no abstract for this session.

Experimental report

There is currently no experimental report.

Experimental data

The data are under embargo until 2021 but could be released earlier. Currently, they are only accessible to proposal team members.

Access data

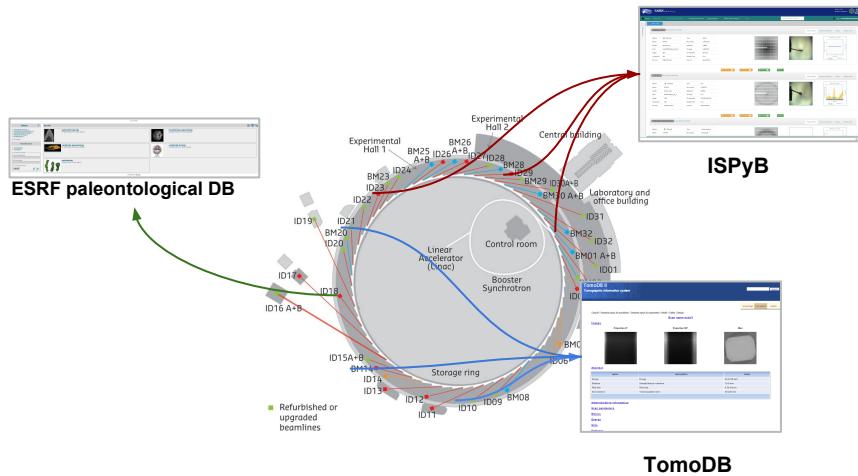
Citation

Below is the recommended format for citing this work in a research publication.

Fedorov R., Machtens D., Reindl T., Cramer J., Reinke P. (2018). Proteins and protein/DNA/RNA complexes involved in biosynthesis, protein folding and degradation, splicing, cancer, host pathogen interacti. European Synchrotron Radiation Facility (ESRF). doi:10.15151/ESRF-ES-115451959



Applications at the ESRF



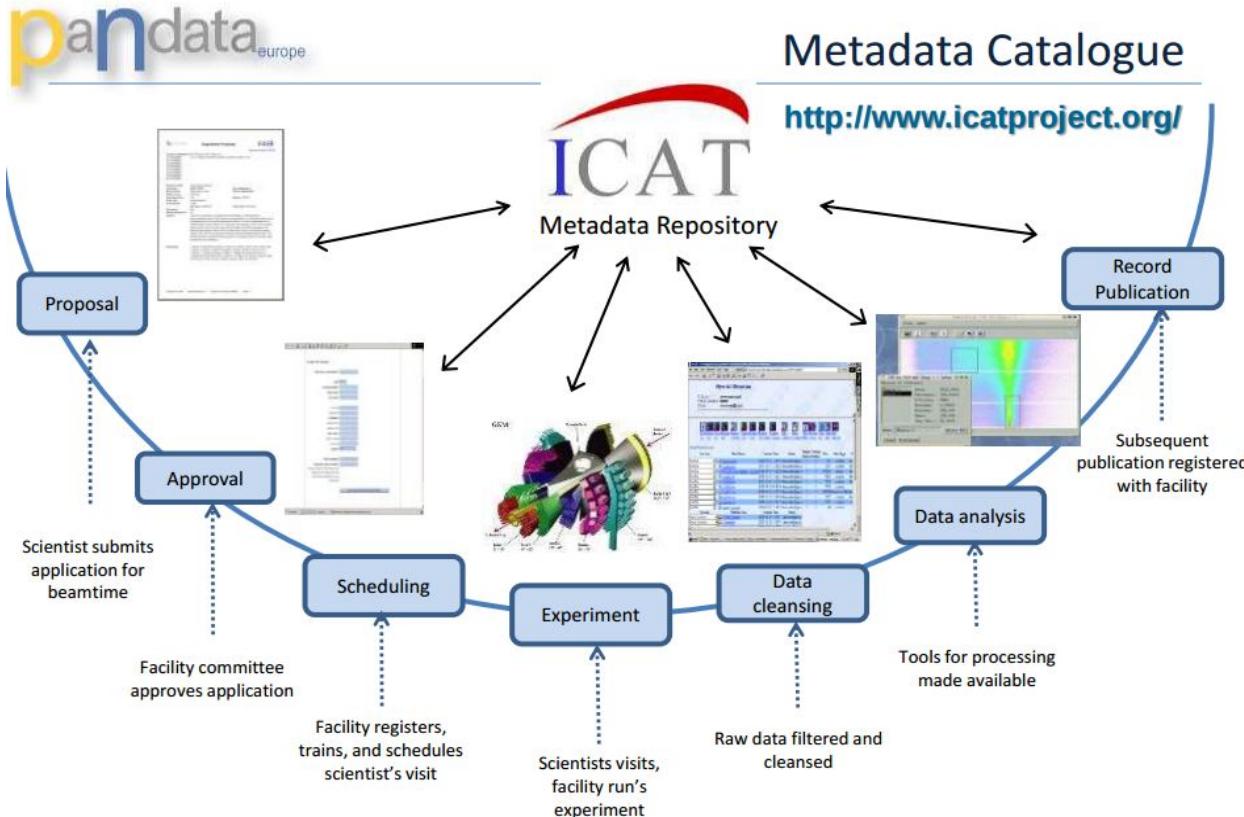
- **Raw Data**

- Data are deleted from disk after 50 days
- Full backups are kept for 2 years
- No data management plan
- No persistent identifiers

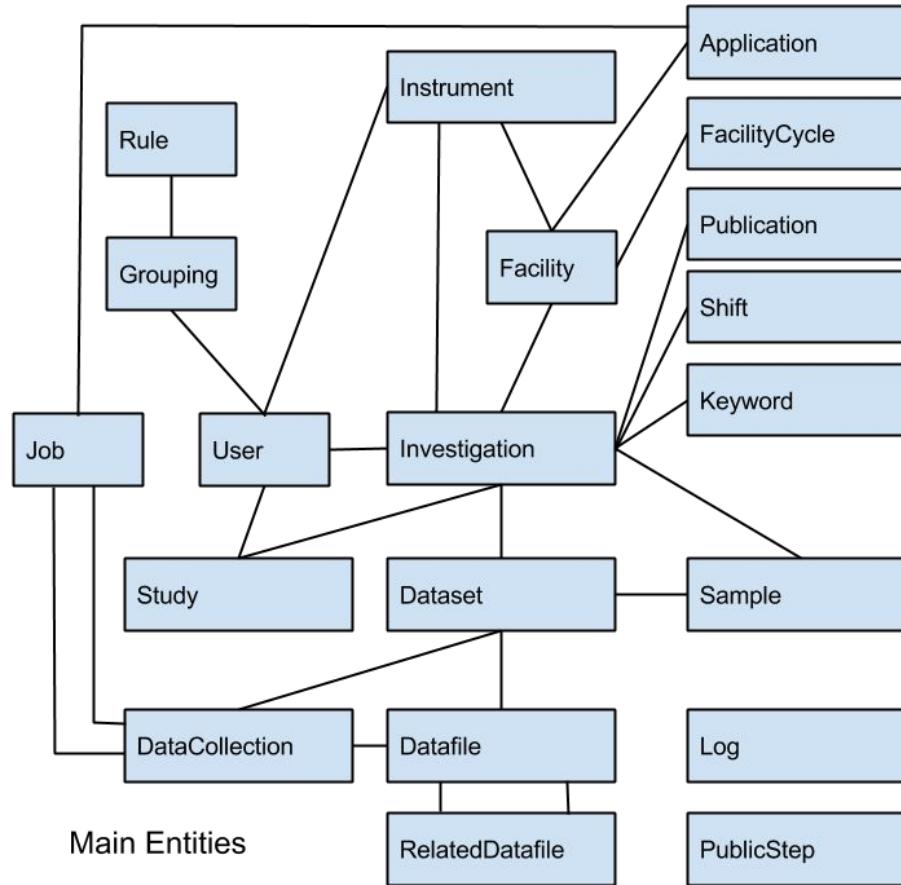
- **Metadata**

- Not collected systematically
- No online metadata catalogue for all beamlines
- Experiment report is not public

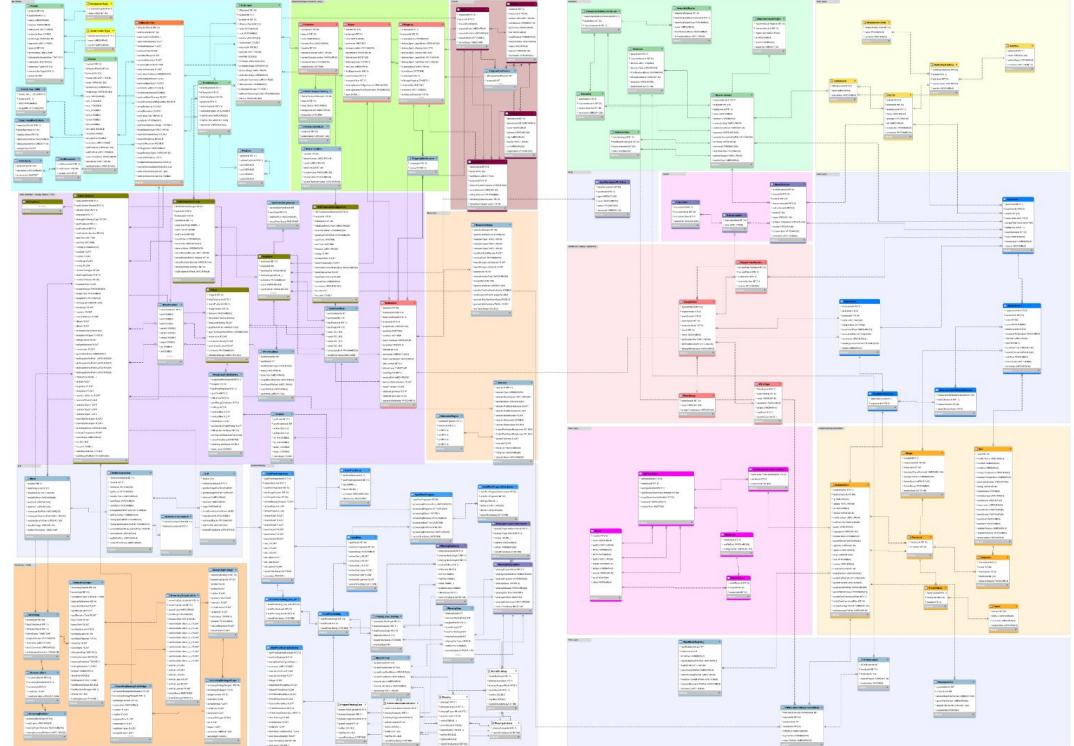
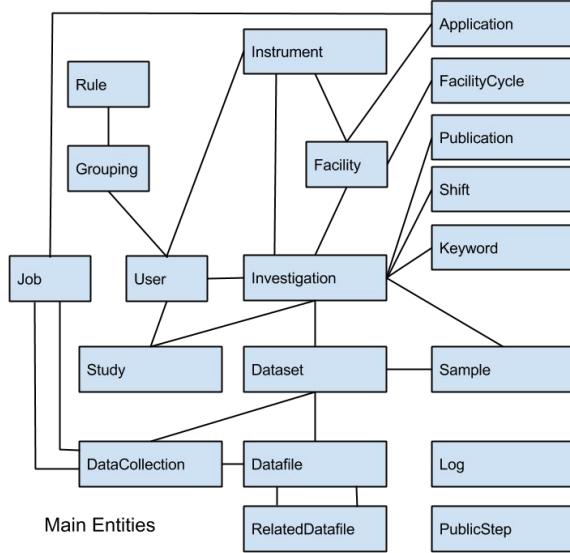
- ICAT is an open source metadata management system designed for **large facilities**



Implementation Overview



Implementation Overview





NXroot

Top level. One per file.

NXentry

One group per measurement

NXinstrument

Describe the instrument.

Only one per NXentry

measurement (@NXcollection)

Flattened view of everything measured

Only one per NXentry

sample (@NXsample)

Define the physical state of the sample

during the scan

NXdata

The data to be plotted.

One NXdata group per plot

user (@NXuser)

Details of a user, i.e., name, affiliation, email address, etc

NXsubentry

Data or links to data for particular analysis

- HDF5 as a mirror of ICAT on the local beamline file system
- Following the NEXUS convention

```
-<group NX_class="NXentry" groupName="${entry}">
  <title ESRF_description="Name of the dataset" ESRF_mandatory="Mandatory" NAPIType="NX_CHAR">${scanName}</title>
  <scanNumber ESRF_description="Scan number" ESRF_mandatory="Mandatory" NAPIType="NX_CHAR">${scanNumber}</scanNumber>
  <proposal ESRF_description="Proposal code" ESRF_mandatory="Mandatory" NAPIType="NX_CHAR">${proposal}</proposal>
  <dataset_type ESRF_description="Scan type can be 'step_by_step' or 'continuous'xA;
" NAPIType="NX_CHAR">${scanType}</dataset_type>
  <folder_path ESRF_description="Scan starting date" ESRF_mandatory="Mandatory" NAPIType="NX_CHAR">${location}</folder_path>
  <start_time ESRF_description="Scan starting date" ESRF_mandatory="Mandatory" NAPIType="NX_DATE_TIME">${startDate}</start_time>
  <end_time ESRF_description="Scan ending date" record="final" ESRF_mandatory="Mandatory" NAPIType="NX_DATE_TIME">${endDate}</end_time>
  <definition ESRF_description="Techniques used to collect this dataset" NAPIType="NX_CHAR">${definition}</definition>
+<group NX_class="NXsubentry" groupName="SAXS"></group>
+<group NX_class="NXsubentry" groupName="MX"></group>
+<group NX_class="NXsubentry" groupName="PTYCHO"></group>
+<group NX_class="NXsubentry" groupName="FLUO"></group>
+<group NX_class="NXsubentry" groupName="TOMO"></group>
+<group NX_class="NXsubentry" groupName="MRT"></group>
+<group NX_class="NXsubentry" groupName="HOLO"></group>
+<group NX_class="NXsubentry" groupName="WAXS"></group>
+<group NX_class="NXsample" groupName="sample"></group>
+<group NX_class="NXinstrument" groupName="instrument"></group>
+<group NX_class="NXnote" groupName="notes"></group>
</group>
```

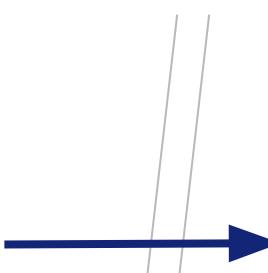
```
-<group NX_class="NXentry" groupName="${entry}">
  <title ESRF_description="Name of the dataset" ESRF_mandatory="Mandatory" NAPItpe="NX_CHAR">${scanName}</title>
  <scanNumber ESRF_description="Scan number" ESRF_mandatory="Mandatory" NAPItpe="NX_CHAR">${scanNumber}</scanNumber>
  <proposal ESRF_description="Proposal code" ESRF_mandatory="Mandatory" NAPItpe="NX_CHAR">${proposal}</proposal>
  <dataset_type ESRF_description="Scan type can be 'step_by_step' or 'continuous'" ESRF_mandatory="Mandatory" NAPItpe="NX_CHAR">${scanType}</dataset_type>
  <folder_path ESRF_description="Scan starting date" ESRF_mandatory="Mandatory" NAPItpe="NX_CHAR">${location}</folder_path>
  <start_time ESRF_description="Scan starting date" ESRF_mandatory="Mandatory" NAPItpe="NX_DATE_TIME">${startDate}</start_time>
  <end_time ESRF_description="Scan ending date" record="final" ESRF_mandatory="Mandatory" NAPItpe="NX_DATE_TIME">${endDate}</end_time>
  <definition ESRF_description="Techniques used to collect this dataset" NAPItpe="NX_CHAR">${definition}</definition>
+ <group NX_class="NXsubentry" groupName="SAXS"></group>
+ <group NX_class="NXsubentry" groupName="MX"></group>
+ <group NX_class="NXsubentry" groupName="PTYCHO"></group>
+ <group NX_class="NXsubentry" groupName="FLUO"></group>
+ <group NX_class="NXsubentry" groupName="TOMO"></group>
+ <group NX_class="NXsubentry" groupName="MRT"></group>
+ <group NX_class="NXsubentry" groupName="HOLO"></group>
+ <group NX_class="NXsubentry" groupName="WAXS"></group>
-<group NX_class="NXsample" groupName="sample">
  <name ESRF_description="Name of the sample" ESRF_mandatory="Mandatory" NAPItpe="NX_CHAR">${Sample_name}</name>
  <description ESRF_description="Description of the sample" NAPItpe="NX_CHAR">${Sample_description}</description>
  <chemical_formula ESRF_description="Chemical formula of the sample" NAPItpe="NX_CHAR">${Sample_chemical_formula}</chemical_formula>
-<group NX_class="NXpositioner" groupName="positioners">
  <name NAPItpe="NX_CHAR">${SamplePositioners_name}</name>
  <value NAPItpe="NX_CHAR">${SamplePositioners_value}</value>
</group>
-<group NX_class="NXenvironment" groupName="environment">
  -<group NX_class="NXsensor" groupName="sensors" ESRF_description="Parameters for controlling external conditions">
    <name NAPItpe="NX_CHAR">${SampleEnvironmentSensors_name}</name>
    <value NAPItpe="NX_CHAR">${SampleEnvironmentSensors_value}</value>
  </group>
</group>
</group>
+ <group NX_class="NXinstrument" groupName="instrument"></group>
+ <group NX_class="NXnote" groupName="notes"></group>
</group>
```

The screenshot shows the ICAT interface with two main panes. The left pane displays the hierarchical structure of an HDF5 file named 'ev325-CG_summer-CG_summer.h5'. The root node is 'entry_0000: CG_summer'. It contains several groups: MX, definition, end_time, folder_path, instrument, measurement, proposal, and source. The 'instrument' group is expanded, showing attenuator, detector01, detector02, insertion_device, monochromator, and optics. The 'measurement' group is also expanded, showing files and proposal. The right pane is a 'Text View' showing a list of 45 measurement files. Each file entry includes a number from 0 to 45, the path to the file, and the file name.

File Number	File Path	File Name
0	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0025_0000_0000.edf	
1	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0131.edf	
2	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0170.edf	
3	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0187.edf	
4	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0018.edf	
5	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0052_0000_0000.edf	
6	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0024.edf	
7	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0105.edf	
8	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0181.edf	
9	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0038_0000_0000.edf	
10	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0090.edf	
11	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0083.edf	
12	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0076.edf	
13	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0187.edf	
14	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0096.edf	
15	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0026_0000_0000.edf	
16	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0130.edf	
17	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0160.edf	
18	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0012_0000_0000.edf	
19	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0042.edf	
20	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0038.edf	
21	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0172.edf	
22	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0137.edf	
23	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0194.edf	
24	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0097.edf	
25	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0027_0000_0000.edf	
26	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0164.edf	
27	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0119.edf	
28	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0109.edf	
29	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0009.edf	
30	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0059.edf	
31	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0113.edf	
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34	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0045_0000_0000.edf	
35	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0171.edf	
36	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0034_0000_0000.edf	
37	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0006_0000_0000.edf	
38	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0137.edf	
39	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0164.edf	
40	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0021.edf	
41	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xmap_x2c_00_0001_0000.edf	
42	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0006.edf	
43	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0000.edf	
44	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0022_0000_0000.edf	
45	/data/visitor/ev325/id21/CG_summer/CG_summer.hires1/zap/CG_summer_hires1/xia0_0001_0000_0086.edf	

Software involved in Data Management

BEAMLINE



CENTRAL
SERVICE



ICAT

```
1956.RH> mdatanewproposal MD7890 /data/id01/{}metadata  
1984.RH> mdata_set_sample("CdTe","kmap", "test of CdTe sample")  
1986.RH> mdata_start "datasetName"
```

```
1986.RH> mdata_put("AcquisitionMode", "Transmission")  
1986.RH> mdata_put("Element", "Fe")  
1986.RH> mdata_put("Edge", "K")  
1986.RH> mdata_upload("saxs", "/data/visitor/../XAS.png")  
  
1986.RH> mdata_save
```

SPEC

- Data is preserved at least 10 years
- Metadata is stored forever
- DOI
- Web Portal
- Electronic Logbook
- Open Data compliant with ESRF data Policy

Search

Name	Beamline	Title	Datasets	Size	Date	Release	
• IH-HC-3376	ID01	Kmapping of Ge microdisks	2128	87 GB		09/03/2021	DOI 10.5072/TEST-ESRF-ES-816112
• MX-2022	BM29	SAXS Characterisation of cationic solid lipid nanoparticles (SLN) in the presence of a cationic surfactant (DDAC)	9485	18 GB	14/12/2017	15/12/2020	DOI 10.5072/TEST-ESRF-ES-792638
• MX-1931	ID23-2	Southampton, UCL Royal Free, Exeter, Portsmouth Block Allocation Group (BAG)	9141	79 GB	14/12/2017	13/05/2021	DOI 10.5072/TEST-ESRF-ES-792638
• MX-1819	ID29	Integrated Ligand Screening Pipelines	4617	4 GB	13/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-777531
• IX-74	ID30B	Helixbiostructures for Morphic Therapeutics samples	362	87 GB	13/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-777179
• IX-78	ID30B	Helixbiostructures for Genzyme Framingham	5010	21 GB	13/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-777090
• IX-71	ID30B	Helixbiostructures for Venenum samples	6183	91 GB	13/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-776355
• IH-CH-1336	ID16A	Characterization of porous and structured materials	9207	92 GB	13/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-774842
• MX-1934	ID23-2	Macromolecular Crystallography BAG - Portugal	754	50 GB	13/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-774842
• MX-2008	BM29	Investigation into the inter-domain linker region and flexibility of the ubiquitin binding protein STAM2: Combined SAXS & NMR approach	3614	61 GB	13/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-774806
• MX-1835	ID30A1	Structure elucidation of light responsive, signal transducing and metalloproteins	5557	96 GB	12/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-771436
• IX-62	ID29	Human α -amino- β -carboxymuconate- ϵ -semialdehyde decarboxylase (ACMSD)	1250	88 GB	12/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-770864
• IN-708	BM05	microtomography analysis of organic materials	4989	52 GB	12/12/2017	21/02/2028	DOI 10.5072/TEST-ESRF-ES-770600
• MX-1949	ID29	Understanding the 3D structure of a variety of proteins related to the human health	2711	8 GB	12/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-769909
• MX-1906	ID23-2	Structural Biology in Marseille	5969	42 GB	12/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-769851
• MX-1862	BM29	Russian Grant Proposal: Study the Spatial Organization of Eukaryotic architectural proteins from D.melanogaster and their complexes	7873	9 GB	12/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-769799
• MX-1862	ID30B	Russian Grant Proposal: Study the Spatial Organization of Eukaryotic architectural proteins from D.melanogaster and their complexes	1038	55 GB	11/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-766218
• MX-1947	ID30B	The London Cancer BAG comprising the ICR, the University of Susses and the Francis Crick Institute	2080	18 GB	11/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-765115
• MX-1947	ID30A3	The London Cancer BAG comprising the ICR, the University of Susses and the Francis Crick Institute	616	71 GB	11/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-763557
• IX-68	ID30B	Helixbiostructures for Warp Drive Bio samples	1458	72 GB	09/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-757600
• IX-69	ID30B	Helixbiostructures for Shire samples	3336	57 GB	09/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-756656
• MX-1862	ID29	Russian Grant Proposal: Study the Spatial Organization of Eukaryotic architectural proteins from D.melanogaster and their complexes	972	99 GB	09/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-755176
• LS-2702	ID16A	Revealing brain nanostructure for better MRI biophysical model	8086	56 GB	08/12/2017	15/02/2028	DOI 10.5072/TEST-ESRF-ES-748589
• MX-1937	ID23-2	Munich Crystallography BAG	7261	1 GB	08/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-748540
• MX-1940	BM29	BAG Paris Rive-Gauche	3652	69 GB	08/12/2017	22/02/2028	DOI 10.5072/TEST-ESRF-ES-748368



⌚ 5:06 AM
December 14, 2017

EXAFS

 vpo_catalyst_prist_60nm_4_ /data/id16a/inhouse1/commissioning/comm_17dec/ihch1336/id16a/vpo_catalyst_prist/vpo_catalyst_prist_60nm_4_[Summary](#) [EXAFS](#) [Metadata List](#) [Files](#)

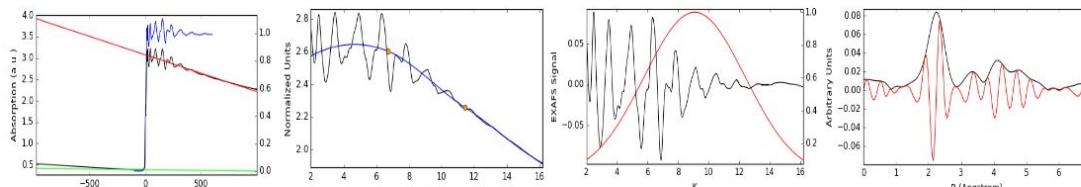
Name vpo_catalyst_prist_60nm_4_

Ac. Mode Transmission

Element Fe

Edge K

Start 5:06:00 AM



Mint a DOI

22 files (46 GB)

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⌚ 4:07 AM
December 14, 2017

EXAFS

 vpo_catalyst_prist_60nm_3_ /data/id16a/inhouse1/commissioning/comm_17dec/ihch1336/id16a/vpo_catalyst_prist/vpo_catalyst_prist_60nm_3_

⌚ 3:10 AM
December 14, 2017

EXAFS

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⌚ 2:13 AM
December 14, 2017

EXAFS

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⌚ 1:05 AM
December 14, 2017

EXAFS

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⌚ 12:06 AM
December 14, 2017

EXAFS

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⌚ 11:09 PM
December 13, 2017

EXAFS

 vpo_catalyst_prist_120nm_2_ /data/id16a/inhouse1/commissioning/comm_17dec/ihch1336/id16a/vpo_catalyst_prist/vpo_catalyst_prist_120nm_2_

⌚ 10:12 PM
December 13, 2017

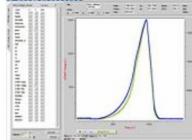
EXAFS

 vpo_catalyst_prist_120nm_1_ /data/id16a/inhouse1/commissioning/comm_17dec/ihch1336/id16a/vpo_catalyst_prist/vpo_catalyst_prist_120nm_1_

E-Logbook

Home ★ My Selection Log out mchaille

did a calibration run of voltage versus temperature on the ETMT. The voltage was read using the Keithley connected as pico1 in the second hutch :

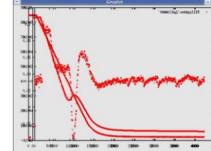


wrote an imagej macro to convert EDF files to an AVI movie. The macro is called EdfMovie. You can find it in :
◦ /data/opid11/inhouse/fable/image/macos/EdfMovie/EdfMovie.txt

Here is an example of calling it :

```
macro 'C3_MakeMovies' {
    runMacro('/data/opid11/external/me1015/scripts/EdfMovie/EdfMovie.txt','//data/opid11/external/me1015/C3_05_con_/,0,1950,10,512,512');
    runMacro('/data/opid11/external/me1015/scripts/EdfMovie/EdfMovie.txt','//data/opid11/external/me1015/C3_10_con_/,0,619,10,512,512');
    runMacro('/data/opid11/external/me1015/scripts/EdfMovie/EdfMovie.txt','//data/opid11/external/me1015/C3_20_con_/,0,819,10,512,512');
    runMacro('/data/opid11/external/me1015/scripts/EdfMovie/EdfMovie.txt','//data/opid11/external/me1015/C3_30_con_/,0,629,10,512,512');
    runMacro('/data/opid11/external/me1015/scripts/EdfMovie/EdfMovie.txt','//data/opid11/external/me1015/C3_40_con_/,0,4810,10,512,512');
    runMacro('/data/opid11/external/me1015/scripts/EdfMovie/EdfMovie.txt','//data/opid11/external/me1015/C3_50_con_/,0,954,10,512,512');
}
```

a quick and easy way to plot the etmt log file is to use gnuplot
◦ type gnuplot and then the following commands
◦ set multiplot
◦ plot 'etmt.log' using 1:8
◦ plot 'etmt.log' using 1:9
◦ plot 'etmt.log' using 1:10
the output looks something like this :



latest version of the me1015.mac macro with the movie macro :

```
# ME1015 - macros for the me1015 experiment
#
def me1015_snap '{
```

European Synchrotron Radiation Facility

E-Logbook

ESRF Home My Selection 0 Log out mchaille

Dataset List 73 Logbook

+ New PDF See as : List Doc

Sep 7

09:48:37 User comment did a calibration run of voltage versus temperature on the ETMT. The voltage was read using the K...
09:48:15 User comment wrote an imagej macro to convert EDF files to an AVI movie. The macro is called EdtMovie. You can fi...
09:48:00 User comment a quick and easy way to plot the etmt log file is to use gnuplot type gnuplot and then the following
09:46:31 User comment latest version of the me1015.mac macro with the movie macro : ## ME1015 - macros for the me1015.edt

09:45:44 User comment

No tags

Write a title here (optional)

Formats

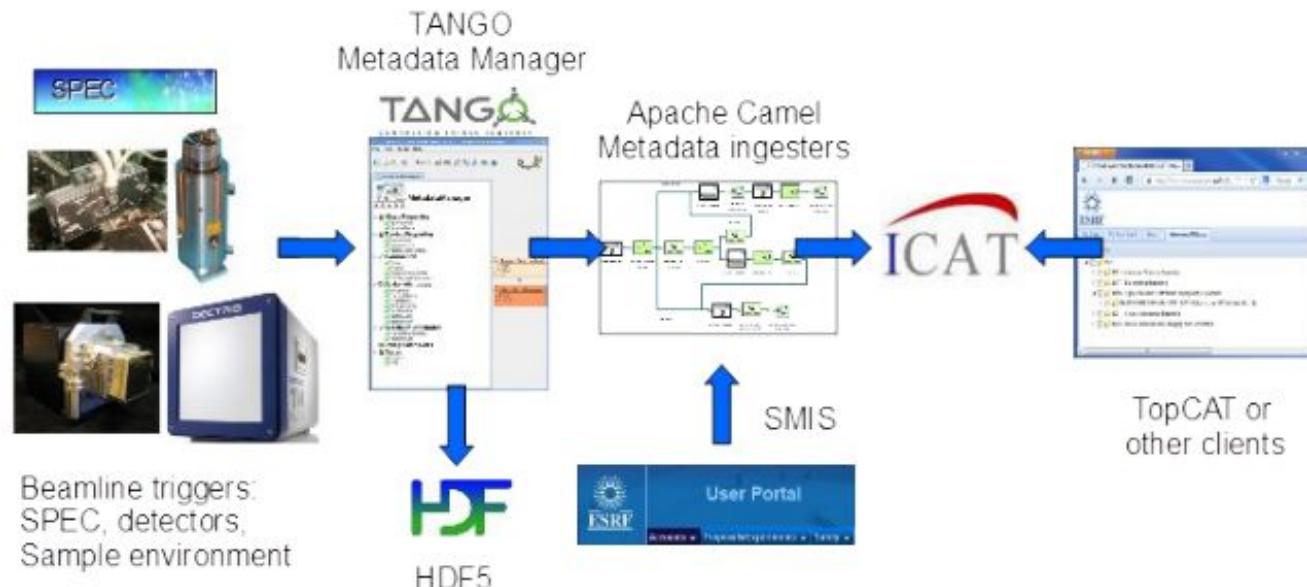
- wrote a new macro called **me1015.movie** which will start an acquisition and read the etmt every 20 ms. When the acquisition is finished the etmt values are written to a log file **etmt.log** for offline correlation with the images times
- I had to modify the espia library **libcodeespia.a** to add high resolution **Frelon2k**
- The **me1015.movie** macro needs to have **Number of Images** set to a number which will cover the duration of the process being recorded. It also needs **on-the-fly** data file saving switched on and the directory and prefix and file number set correctly. NOTE that you MUST type return in each window when you change a value.
- The on-the-fly gui window looks like this :

Save Cancel

09:45:05 User comment tried to program the camera mode, kinetics etc at the beginning of each scan but it caused the devic...

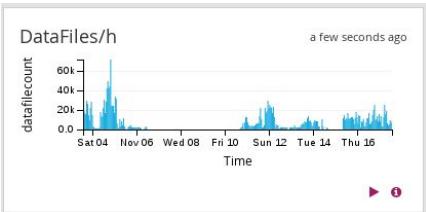
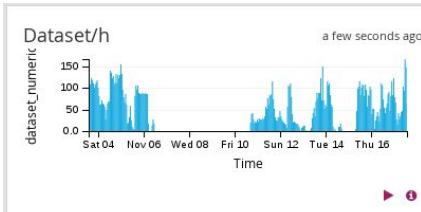
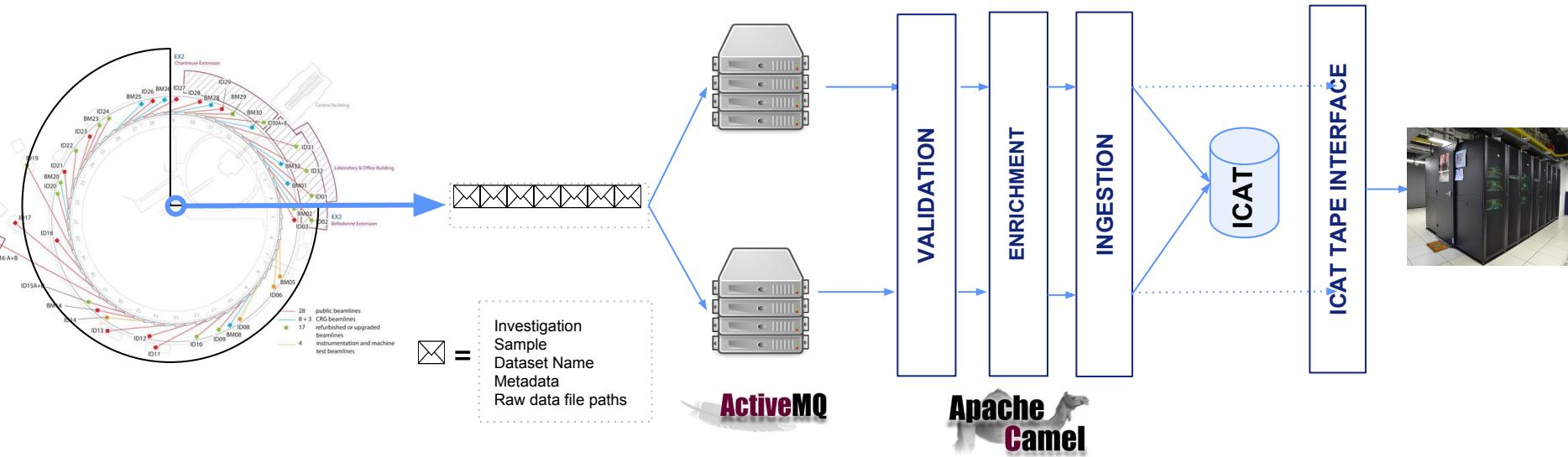
09:43:55 User comment Log Andy 09:00, 5 March 2006 (CET) started up did some tests on the Frelon to see how fast we can...

09:43:17 User comment Motors Following motors are useful : zb - z beam stop x2 - x ccd camera y1 - y stress rig + ccd ca...



Architecture

<https://icat.esrf.fr>



PRODUCERS

CONSUMERS

Status(<http://www.esrf.fr/datapolicy>)

Data Policy Implementation					
Beamline Status	Techniques	Metadata Collection*	Data archiving*	Raw Data in HDF5*	Open access to data*
ID01	KMAP	Implemented	Implemented	In progress	
BM01A					
BM01B					
ID02					
BM02					
ID03					
BM05	Tomography	In progress	In progress	In progress	
ID06-LVP					
ID06					
BM08					
ID09					
ID10					
ID11	Tomography	In progress	In progress	In progress	
ID12					
ID13					
BM14					
ID15A					
ID15B					
ID16A	Fluo, Tomo	Implemented	Implemented	In progress	
ID16B	Tomo	In progress	In progress	In progress	
ID17	MRT, Tomography	Implemented	Implemented	In progress	
ID18					
ID19	Tomography	In progress	In progress	In progress	
ID20 ↴	RIXS	In progress	In progress		
ID21	Microscopy	Implemented	Implemented		
ID22					
ID23-1	MX	Implemented	Implemented	In progress	
ID23-2	MX	Implemented	Implemented	In progress	
BM23					

ID24					
BM25A					
BM25B					
ID26					
BM26A					
BM26B					
ID27					
ID28					
BM28					
ID29	MX	Implemented	Implemented		In progress
BM29	BIOSAXS	Implemented	Implemented		In progress
ID30A-1	MX	Implemented	Implemented		In progress
ID30A-3	MX	Implemented	Implemented	Implemented	In progress
ID30B	MX	Implemented	Implemented		In progress
BM30A					
BM30B					
ID31					
ID32	RIXS	In progress	In progress		In progress
BM32					
CryoEM	Single Particle	Implemented	Implemented		In progress

***Techniques covered** - lists which techniques are currently concerned by the Data Policy

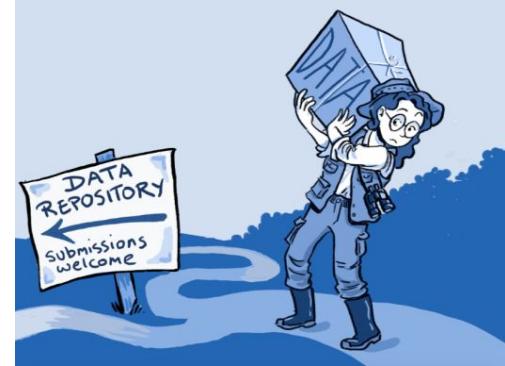
***Metadata collection** - status of metadata collection and storage in metadata catalogue for the listed techniques (orange = planned / in progress, green = implemented, grey = not planned / implemented yet)

***Data archiving** - status of long term archiving in tape library (green = data are being archived for 10 years in tape archive)

***Open access of data** - indicates if data is open access (green) or still under embargo (red), or no data archived (grey)

Implementation Coordination Team Members

- Alejandro de Maria (ISDD) – Data Manager
- Bruno Lebayle (TID) – IT infrastructure
- Joanne McCarthy (EXPD) – User Office
- Armando Solé (ISDD) – Metadata+data
- Jens Meyer (ISDD) – Beamline controls
- Dominique Porte (TID) – User ID's
- Rudolf Dimper (TID) – Data policy
- Andy Götz (ISDD) – Implementation



Thanks for your attention!!