

Data Management at ILL.

Experimental data evolution and its consequences.

Presentation given at the CREMLIN workshop on Big data Management

16th of Feb 2017 NRC “Kurchatov Institute” - Jean-François Perrin (ILL IT Services) / Jiri Kulda (ILL/Science Dpt)

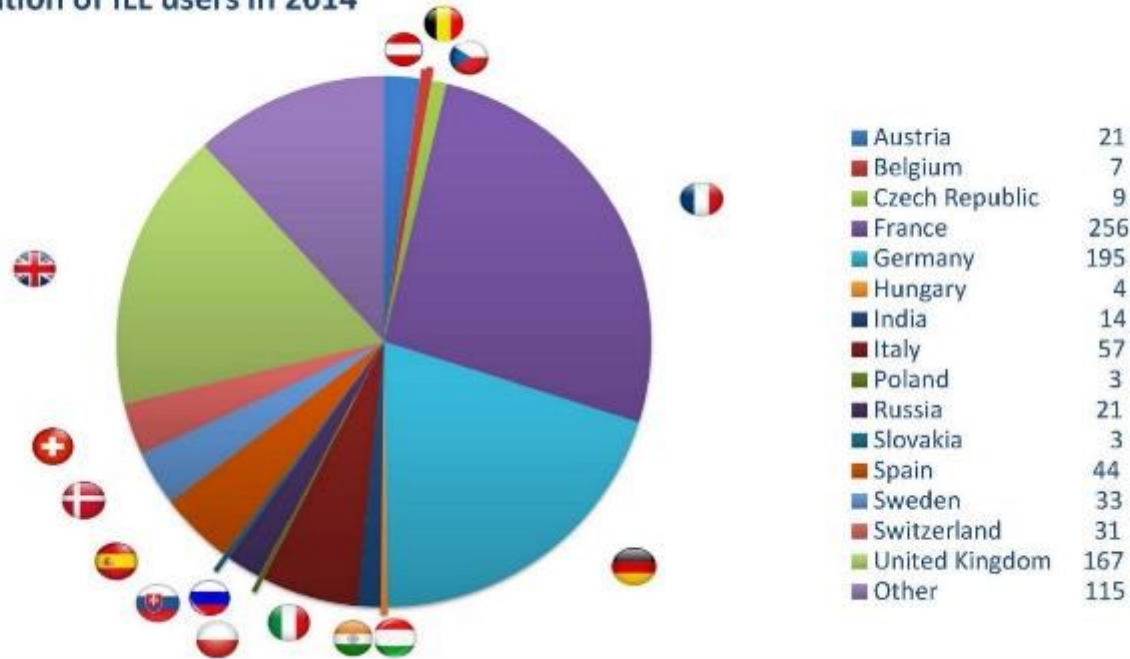
Short introduction to the ILL

Users

An active community of 12 000 scientists from 28 countries

1400 invited experimenters / year

National affiliation of ILL users in 2014





Users are travelling

Snapshots of unique X-Ray & Neutron scattering users, over 18 months (2013 – 2014).

	ALBA	BERII	BESSYII	DESY	DLS	ELETTRA	ESRF	MLZ	ILL	ISIS	LCLS	SINQ	SLS	SOLEIL	SNS	neutron	photon	all
ALBA	1303	5	43	90	274	128	356	8	83	36	2	23	124	161	7	122	679	1303
BER II	5	237	27	28	20	0	42	66	104	50	0	75	22	7	37	162	86	237
BESSY II	43	27	838	128	96	95	143	16	31	16	28	29	119	100	11	76	418	838
DESY	90	28	128	3680	396	255	901	110	167	92	151	82	326	246	63	343	1579	3680
DLS	274	20	96	396	10445	297	1606	82	485	763	70	144	559	526	124	1136	2598	10445
ELETTRA	128	0	95	255	297	3422	480	21	99	41	68	14	218	379	12	149	1171	3422
ESRF	356	42	143	901	1606	480	10786	203	731	356	102	203	899	1390	155	1165	4242	10786
MLZ	8	66	16	110	82	21	203	1430	409	167	3	222	52	46	158	601	353	1430
ILL	83	104	31	167	485	99	731	409	4138	606	3	384	130	239	316	1252	1304	4138
ISIS	36	50	16	92	763	41	356	167	606	3406	9	236	101	84	267	891	1052	3406
LCLS	2	0	28	151	70	68	102	3	3	9	1123	1	79	44	6	17	329	1123
SINQ	23	75	29	82	144	14	203	222	384	236	1	1424	250	65	185	614	501	1424
SLS	124	22	119	326	559	218	899	52	130	101	79	250	3981	366	64	365	1637	3981
SOLEIL	161	7	100	246	526	379	1390	46	239	84	44	65	366	5134	40	349	2145	5134
SNS	7	37	11	63	124	12	155	158	316	267	6	185	64	40	3723	581	327	3723

ILL member countries and their financial participation



Germany : 25 %

UK : 25 %

France : 25 %

Spain

Italy

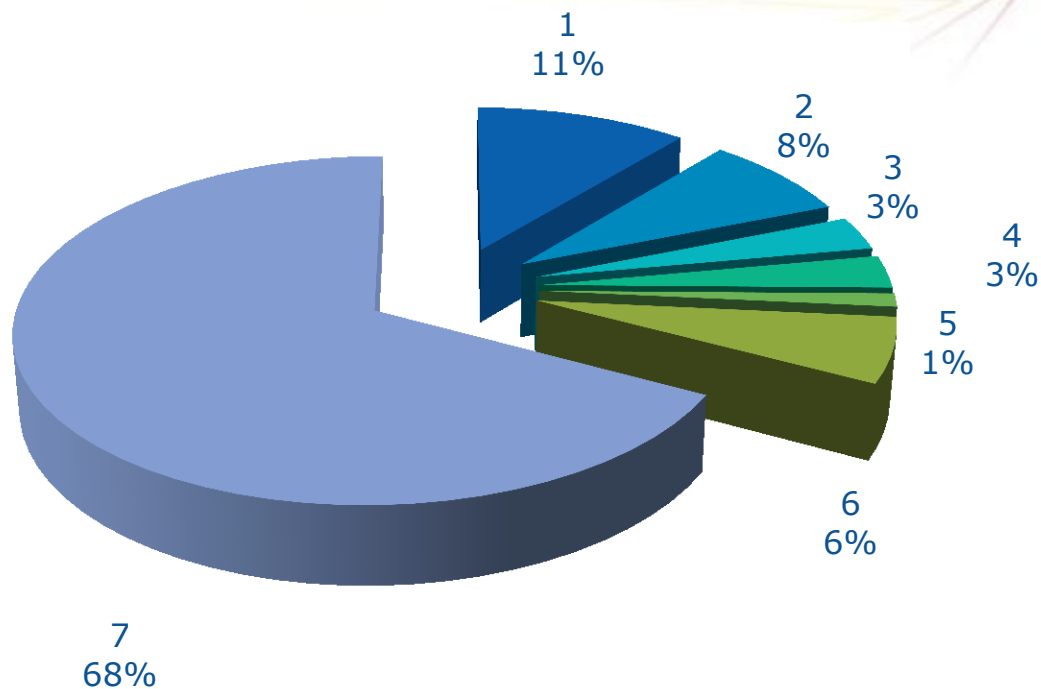
Switzerland

Poland

CENI (Central European Neutron Initiative,
Austria, Czech Republic, Slovakia)

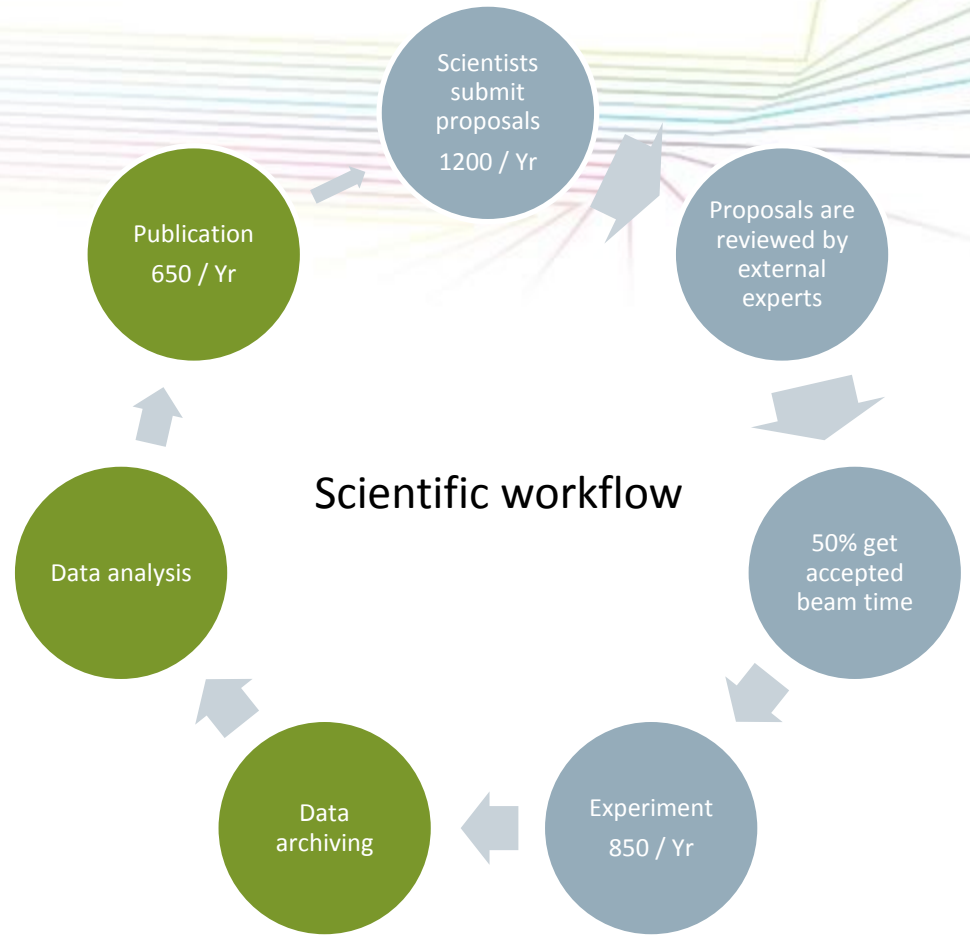
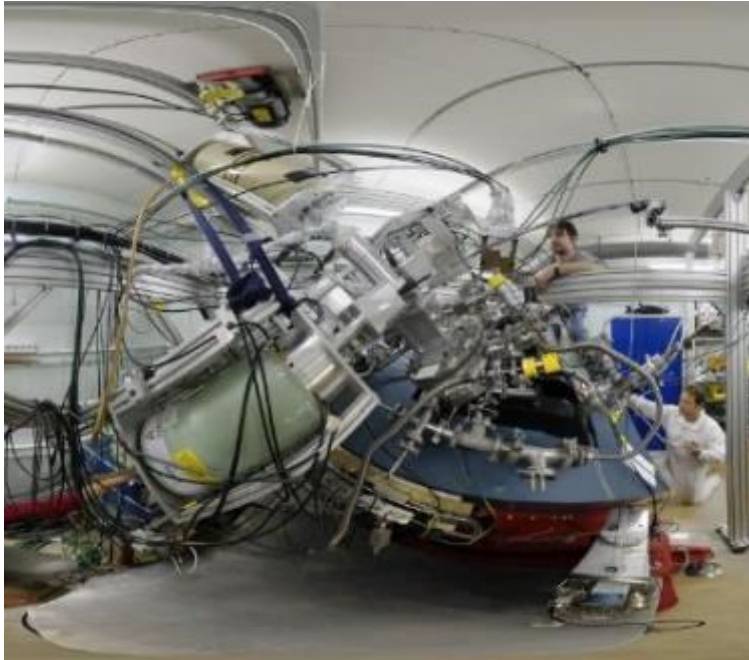
TRANSNI (TRANSnational Neutron Initiative,
Belgium, Denmark, Sweden)

Societal impact



Science

28 instruments + 10 CRG



Instruments

Organised in 4 groups

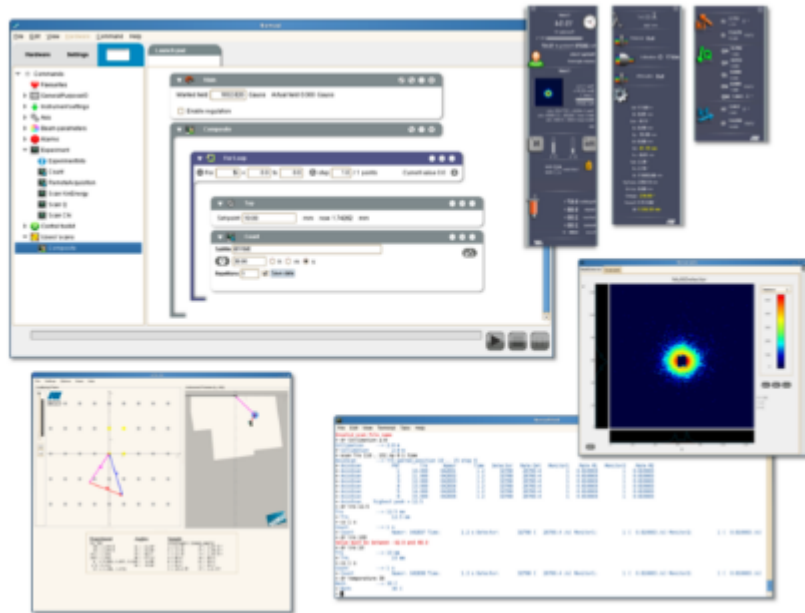
- Spectroscopy:
 - Time-of-flight spectrometers
 - Backscattering spectrometers
 - Spin-echo spectrometers
 - Three-axis spectrometers
- Diffraction:
 - Powder diffractometers
 - Single-crystal diffractometers
- Large scale structures:
 - Diffractometers
 - Reflectometers
- Nuclear and particle physics



Instrument control

Under the responsibility of DPT/SCI

NOMAD is the ILL's sequencer to control instrument operations.

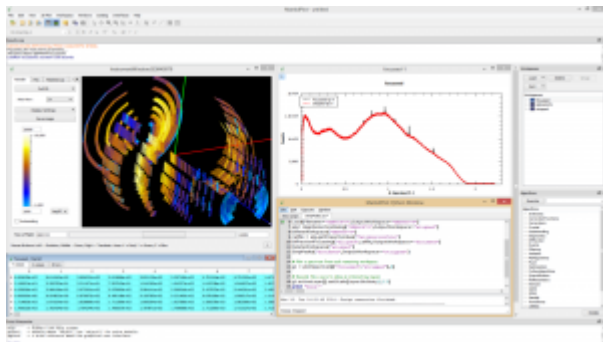


- Allow to control all operations on the instruments.
- Users can build their specific workflows (GUI/drag & drop or CLI/scripting approach)
- Client/server architecture (Java/C++)
- Open sourced under EUPL
- <https://www.ill.eu/instruments-support/instrument-control/software/nomad/>

Data Reduction (future)

Under the responsibility of DS/CS

- Mantid (<http://www.mantidproject.org>)
 - Large worldwide collaboration between Neutron RI: ISIS, SNS & HFIR, ESS, ANSTO, PSI, ILL
 - Mantid was developed for spallation sources. ILL is investing 3-4 FTE over 3 yrs to adapt Mantid to the ILL (reactor source) instrument suite.
<https://www.ill.eu/fr/instruments-support/computing-for-science/data-analysis/mantid-tutorial-ill-resources/>
 - For more info, watch Jon presentation.



Data Analysis

Under the responsibility of DS/CS

- A large set of existing tools

- <http://www.ill.eu/instruments-support/computing-for-science/cs-software/all-software>
- <https://www.ill.eu/sites/fullprof/>
- ...

- WP10 of SINE2020 project

Tech.	Software	Lead (+co.)	Improvements
Imaging	MuRec & KipTool	PSI (+CEA, ISIS, ESS)	Conversion to open source software. More user-friendly interfaces, optimized algorithms for GPU and distributed computing for faster analysis, and new reconstruction algorithms.
Reflectometry	BornAgain	FZJ	Addition of GUI, extension to all types of reflectometry, and algorithms optimized for real time analysis.
SANS	SASView	ESS (+PSI)	Modularization and new GUI. Addition of API and CLI. Optimization of algorithms for real time analysis and extension with SASFit model fittings.
QENS	Mantid	STFC (+ILL, FZJ)	More user-friendly interfaces and extension of model fitting functions.
Atomistic modelling	nMoldyn, DFT	ILL (+ESS, ISIS, PSI, UNIPR)	Extension to convert lattice dynamics and Monte Carlo simulations to scattering curves. Development of muon spectroscopy as a complementary tool for neutron scatterers through improved data analysis exploiting atomistic modelling such as density functional theory (DFT).

SINE2020 WP10 aims

- Convergence to a common set of supported tools by Ris
- Straightforward generation of scientific results for non-expert and industry users.
- Data treatment software ready for users at ESS

Experimental data management



Co-funded by the European Union :

PaNData-Europe Grant Agreement No 261537

PaNData-ODI Grant Agreement No RI-283556

INSTITUT MAX VON LAUE - PAUL LANGEVIN

Open Data/Science for a facility?

- Data are the real/factual production.
- Knowledge (peer-reviewed articles, conference contributions, thematic courses, software ...) is the main output.

Openness is a tool for increasing our **impact**.

What has been done so far?

- 2008 1st discussion on Data Policy (PaNData)
- 2011 “Open” DP published - 3 (max 5) years embargo
- 2012 1st experiment under DP
- 2013 complete set of Data Management Services available for users: search, access, annotate, archive, identify, publish, ...
- since then, communication with our users ...

1) Data Policy

Based on the PaNData framework



Open data & how to protect and credit our users?

- The facility shall act as a custodian for the data.
- All raw data will be curated in a well-defined format with a unique ID (DOI).
- Metadata is captured automatically and resides either within the raw data files, and/or in an associated on-line catalogue.
- Users can release or give access to their data at any time, by default access to raw data and the associated metadata is restricted to the experimental team for a maximum period of 3 years. Thereafter, it will become publicly accessible.
- The embargo period can be extended on request to the ILL management.
- Publication based on data must acknowledge the source of the data and cite its unique identifier (CC-BY licence).

<https://www.ill.eu/DataPolicy>

2) Linking Proposal and data.

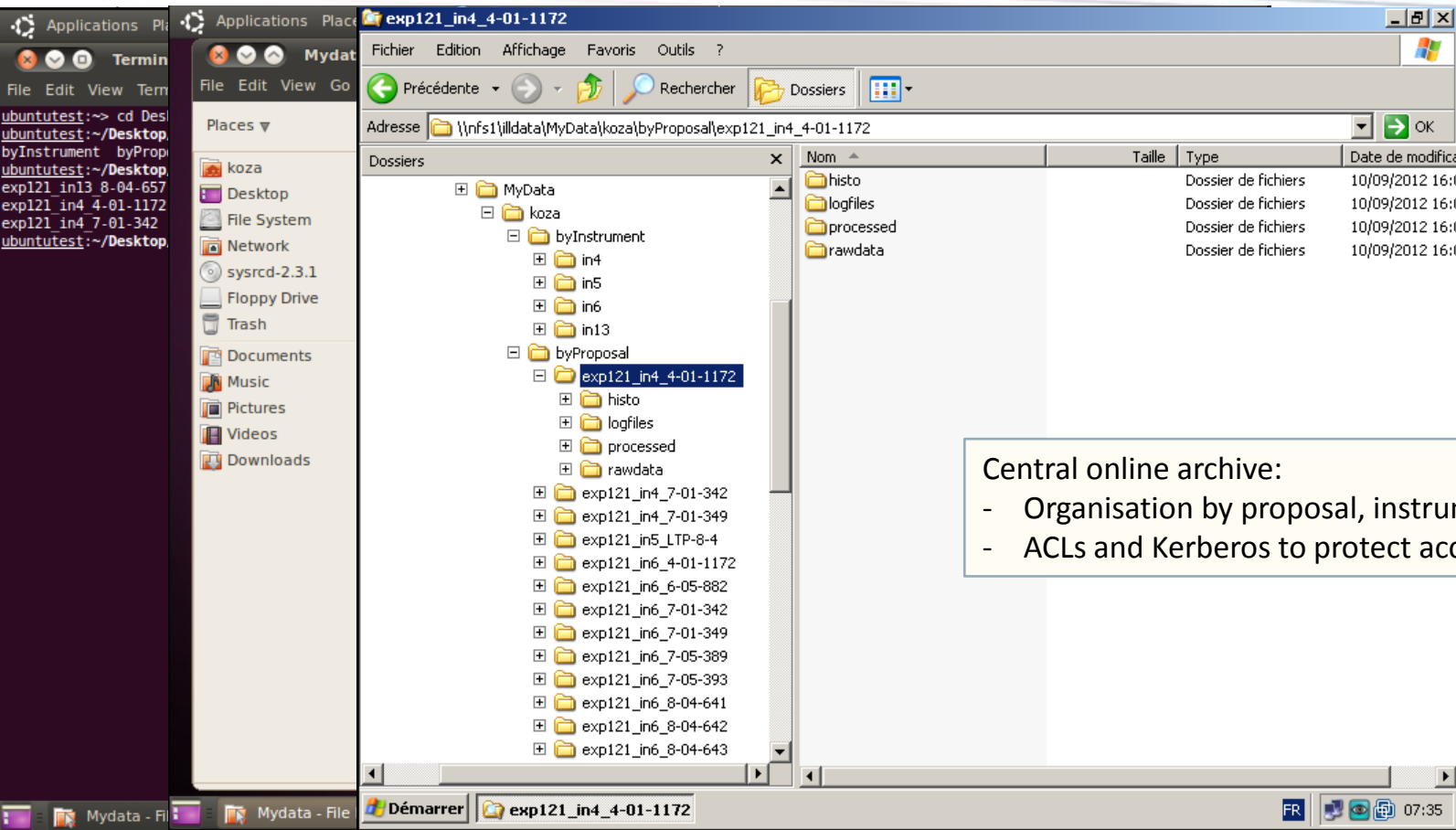
Identification of the proposal on the instrument.

The screenshot displays a software interface for linking a proposal to data on an instrument. The interface is divided into several sections:

- Left Panel (Commands):** A tree view showing various command categories: Favourites, Acquisition, Counts (with sub-items: Count, KineticCount, TotCount, PHKineticCount), Scans, Setting, Title, Axis (with sub-items: Primary, Secondary), Beam parameters, Sample environment, Tools, Execution control, Clipboard, and Users' scripts.
- Central Panel (Hardware Settings):** A panel with tabs for Hardware, Settings, and Execution. It shows settings for different hardware components: Count (Subtitle: D20, Repetitions: 1), Disk3 (Set-point: 270.0), Disk4 (Set-point: 270.0), and another Count (Subtitle: D20, Repetitions: 1).
- Right Panel (Proposal List):** A panel titled "Select a proposal from the list below." It contains a table with two columns: Code and Title. The table lists various proposals, including "Internal use", "Magnetic ordering in Ni-Co-Mn-Si-based ferromagnetic shape memory alloy (FSMA)", "Behaviour of Alkali-Borosilicate glasses under irradiation: A SANS study on the evolution of segregated phases", "Investigation of vortex structures in the intermediate mixed state of dMgB_2 : comparison with Niobium", "Probing magnetic phase separation at a metal-insulator transition", "Clarifying the origin of chain superconductivity in Y-based cuprates: why does $\text{YBa}_2\text{Cu}_4\text{O}_8$ behave differently to $\text{YBa}_2\text{Cu}_3\text{O}_7$ ", "Protic Ionic Liquid 6- β -D-11; Water Interactions", "Combined SANS & NMR studies of seven transmembrane helical proteins in native-like membrane mimetic environment", "Investigation of the role and effect of hydration on an amyloid forming peptide using both high and small-angle neutron scattering", "SANS Investigations on aggregation phenomena in supersaturated drug solutions", "A Neutron Scattering Solution Study of Chromatin Regulatory Proteins in the Human Malaria Parasite", "Interaction of Hyaluronan and Phospholipids", "Structural analysis of the interaction between a polyelectrolyte with protein varying salt concentration and temperature", "Structure of the interaction between complement factor H (CFH) and complement C3d in relation to inflammatory diseases", "Structure in unusual microemulsions", "Tri-chain surfactants as charge control agents for colloids in nonpolar solvents", "Self-assembly of low surface energy surfactants", "Contact ripening of emulsions", "The structure and morphology of mono-, bi-, and tri-layer graphenes in solution as a function of concentration and solvent", and "Concentration induced size and shape changes in ionic microgel systems".

A dialog box is open over the proposal list, showing the "Select" and "Cancel" buttons. The status bar at the bottom indicates "Setting username to internal use".

3) Archive: ACLs & user experience improvements



The image shows a Linux terminal window on the left and a file manager window on the right. The terminal displays a series of commands and their outputs, showing the user navigating through the file system. The file manager window shows a directory tree with the following structure:

- koza
 - Desktop
 - File System
 - Network
 - sysrcd-2.3.1
 - Floppy Drive
 - Trash
 - Documents
 - Music
 - Pictures
 - Videos
 - Downloads
- MyData
 - koza
 - byInstrument
 - in4
 - in5
 - in6
 - in13
 - byProposal
 - exp121_in4_4-01-1172
 - histo
 - logfiles
 - processed
 - rawdata
 - exp121_in4_7-01-342
 - exp121_in4_7-01-349
 - exp121_in5_LTP-8-4
 - exp121_in6_4-01-1172
 - exp121_in6_6-05-882
 - exp121_in6_7-01-342
 - exp121_in6_7-01-349
 - exp121_in6_7-05-389
 - exp121_in6_7-05-393
 - exp121_in6_8-04-641
 - exp121_in6_8-04-642
 - exp121_in6_8-04-643

The file manager window also shows a table of files with columns: Nom, Taille, Type, and Date de modification. The files listed are:

Nom	Taille	Type	Date de modification
histo		Dossier de fichiers	10/09/2012 16:0
logfiles		Dossier de fichiers	10/09/2012 16:0
processed		Dossier de fichiers	10/09/2012 16:0
rawdata		Dossier de fichiers	10/09/2012 16:0

Central online archive:

- Organisation by proposal, instrument, dates.
- ACLs and Kerberos to protect accesses.

Logs from the instrument control and user annotation (text, image, analysis results ...)

Logs from the instrument control and
user annotation (text, image, analysis results ...)

5) Data portal

 **Data Toolbox** Jean-François Perreault
Your tools to manage your ILL Data

- Provide access to data, meta-data, logs, DOIs landing page, ...
- Tools for managing data authZ

- Tailored to ILL needs
 - User management of data access authorization.
 - Users could decide to publish (open access) their data, before the end of the embargo period.

Global Search

n5 quasielastic

☐ Include experiments without data

Advanced Search

My role in the experiment (?)

Proposal number (?)

Proposal title

Proposals list

Proposal 8-24-684

Proposal Members Data ranges Data folders

131n5Sleep_8-04-684

- histo
- logfiles
- rawdata

The screenshot displays the I2D2 database interface. On the left, there is a sidebar with 'Global Search' and 'Advanced Search' sections. The 'Global Search' section shows the search term 'in5 quasielastic' and a checkbox for 'Include experiments without data'. The 'Advanced Search' section has a dropdown for 'My role in the experiment (?)' and a text input for 'Proposal number (?)'. The main content area, titled 'Proposals list', shows a search result for '18 proposal(s) found with the given search filter'. The first result is '8-04-684 : The influence of cofactor binding on thermal fluctuations of alcohol dehydrogenase studied by using quasielastic neutron scattering'. The search criteria are listed as: Title: quasielastic neutron scattering, Abstract: related to the collective domain motions. In this proposal we propose to investigate using the IN5, Data title: quasielastic neutron scattering, and Proposal file: visi. Below this, another result '6-02-512 : Dynamics' is partially visible. At the bottom, a table lists various data files with their IDs and sizes, and a context menu is open over the first few rows, offering options like 'Download files (one by one)', 'Download a zip with all files', and 'Select all files'. A yellow callout box on the right contains the text: 'Index all available information: Proposal, experimental report, data file annotation, publications, ...'. The footer of the page reads 'INSTITUT MAX VON LAUE - PAUL LANGUETZ'.

Global Search

in5 quasielastic

☐ Include experiments without data

Search

Advanced Search

My role in the experiment (?)

Proposal number (?)

Proposals list

18 proposal(s) found with the given search filter

8-04-684 : The influence of cofactor binding on thermal fluctuations of alcohol dehydrogenase studied by using quasielastic neutron scattering

- Title: quasielastic neutron scattering
- Abstract: related to the collective domain motions. In this proposal we propose to investigate using the IN5
- Data title: quasielastic neutron scattering
- Proposal file: visi


6-02-512 : Dynamics

Index all available information: Proposal, experimental report, data file annotation, publications, ...

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6) DOIs

Collaboration
with DataCite
– INIST (French rep)



ILL
NEUTRONS
FOR SCIENCE

DOI > 10.5291/ILL-DATA.9-11-1654

Please note

The full details of this dataset is not yet available to the public as it still under its embargo period. As such there are only a few details publically exposed. To find out more about how the ILL governs the release of data, please go [here](#). Thank you for your understanding

Title

Chitosan/gelatin enzymatically cross-linked hydrogels: Composition and temperature effects on the gels' molecular structure

Abstract

Hydrogels from biopolymers have been attracting increasing interest in biomedicine, but the lack of structural understanding hinders the development of hydrogel scaffolds obtained from the blend of biopolymers like gelatin and chitosan. The hydrogels are cross-linked by the enzymatic cross-linking reaction. The gelation will be studied: (a) Chemical gelation, enzymatic reaction (b) Physical co-chemical gelation, enzymatic reaction done in presence of the hydrogel. In more than the added properties of its components, and it also requires a particular set of mechanical properties, which are related to its application. At the nanoscopic level, we propose to use SANS to achieve an understanding of the structure of the networks at the nano-scale level, both after and during the gelation. The experiments will give us precious insight into hydrogels architecture and properties allowing us to better correlate bulk and nano-properties in order to allow a better understanding of the final hydrogels.

Experimental Report

[Download Experimental Report](#)

Download Data

The data is currently only available to download if you are a member of the proposal team

[Download Data](#)

Data Citation

This data has been cited by 1 articles.

[Exploring the Kinetics of Gelation and Final Architecture of Enzymatically Cross-Linked Chitosan/Gelatin Gels](#)

Marcelo A. da Silva, Franziska Bode, Isabelle Grillo, and Cécile A. Dreiss (2015).

DOI: [10.1021/acs.biomac.5b00205](https://doi.org/10.1021/acs.biomac.5b00205)

Data has been collected on

Authors

da Silva, MA ([ORCID](#), [ResearcherID](#))

DREISS Cecile

Isabelle Grillo

Cycles

20151 (19-02-2013 - 09-04-2013)

Proposal number

9-11-1654

Experiment Parameters

This data is not yet public

Parameters


J.-F. ILL

Institut Laue-Langevin

Copyright © 2015

Access to data is governed by the ILL data policy

ILL has partnered with [DataCite](#) as the registration agency for data persistent identifiers.

 DataCite

Issue #1: Awareness of the scientists

- This is still new for most of the scientists
“What are DOIs? What are you talking about?”
- We currently feel a bit alone – critical mass. (ESRF, PSI, ESS, have recently joined)
- We need more communication – mentoring – cultural change - education.

Need to fill the gap between what we hear in RDA-like meetings and the daily reality of the scientists.

Still need to convince the scientist that a change is happening regarding experimental data.

Issue #2: Difficulty to collect the articles exploiting the experimental data

- Technical reason : DOIs in figures instead of references, partial citations ...
- No tools yet available to easily collect references
 - CrossRef cited by linking - currently only for article (vs data) publishers ? -, OpenAire.
 - This is a business for the publishers.
- Difficulties to get metrics: how successful are we?
 - We have currently (Dec 2016) collected less than 50 peer reviewed article referencing the data DOI.
 - How many are we missing?

Need to access freely information for building metrics.

Issue #3: time

A decorative graphic consisting of numerous thin, curved lines in various colors (yellow, green, blue, purple, pink) that originate from the right side of the slide and fan out towards the left, creating a sense of motion or a network.

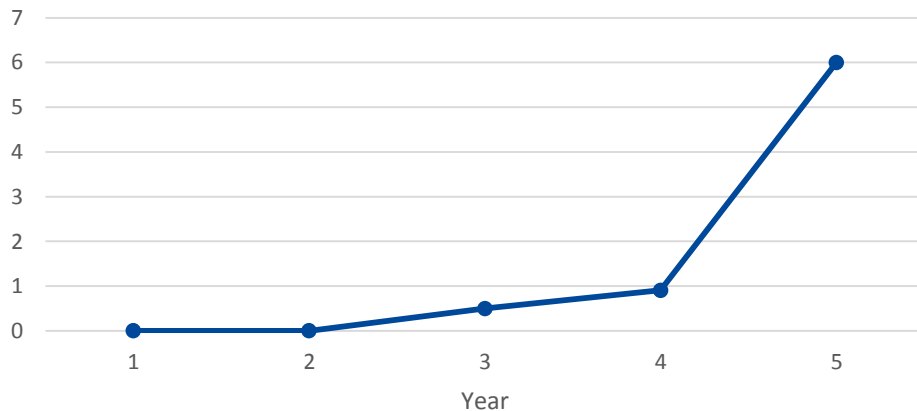
- Time for analyses
- Time for writing articles
- Time for publication
- Time for convincing

This is by nature a long process, but seeing the level of investment needed, we need to convince, we need evidence of success urgently.

Results as of Dec 2016

- Few data sets have been made public by users before the end of the embargo period.
- The reference to Data sets in scientific articles, through DOIs, is recently improving.
- Real interest of the publishers <http://www.elsevier.com/?a=57755>
- More user feedback: "Why I don't get a DOI for experiment XYZ?"

% of ILL users' publication citing the data sets through DOIs

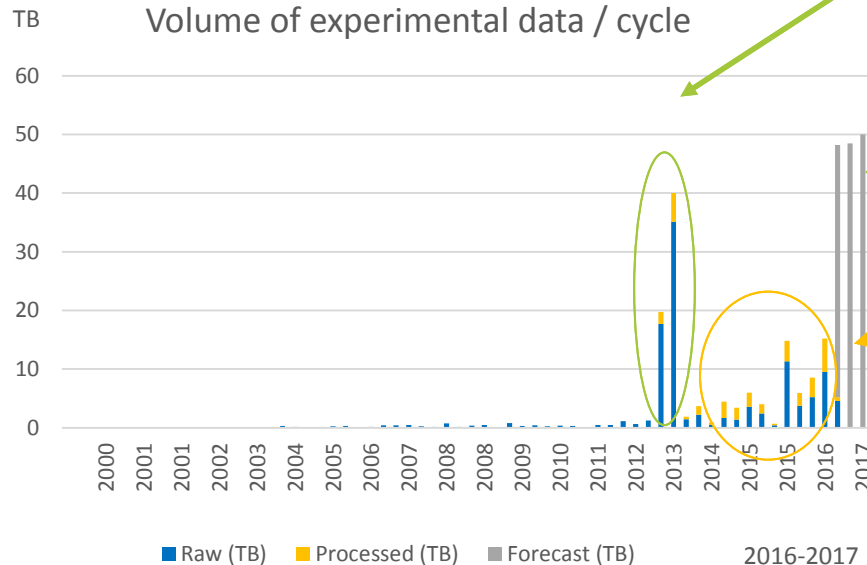


More generally

- Better tools for our users
 - Following remote experiment: live remote access to data, logs, ...
 - Easier access/discovery to data sets.
- Better archiving - from 'bit level' responsibility to 'usability level'.
- New services for users:
 - Ready for Open Data - Some journals (e.g. PLOS) request access to data for every article or for referees.
 - Data Management Plan (more and more mandatory for grant request)

Data Analysis As a Service.

Data volume evolution



Evaluation of new detectors/techniques leading to permanent instruments starting from Jan 2017.

Moving to list mode (vs Histo)

Impacts of the data volume evolution

Example of the EXILL campaign

- Storage (2 experiments = 70TB)
 - ILL archive capacity & performance
 - Users' storage becoming almost impossible
- Moving data
 - Today how to carry 40TB to 10 different labs?
 - Why carrying them?
- Analysis
 - Almost impossible in most users' labs with such data sets.
- But
 - 32 direct (h-index 4) peer reviewed articles published
 - 2 Phd-thesis
 - 10+ international conferences
 - ...



Our vision

- Large raw data sets should be archived at the source (ILL in our case).
- Provide remote analysis infrastructure – data and analysis capacity should be colocated.
- Preserve data and the scientific workflow.
- Most of the analytical facilities face the same problem. We share a large part of our User community. We need to work together: **PaNDaaS**

Data analysis as a Service

- The aim is to proposed to users to access analysis services (**data, software, IT capacity and expertise**) remotely using standard tools (ideally only web browser).
- Typical workflow:
 - 1) The user connects remotely using his web browser and its credentials (Federated IM)
 - 2) Then select one of the experiment he has performed in the list.
 - 3) he is then connected to a service where the necessary analysis applications have been installed and configured for accessing directly the experimental data.
 - 4) If necessary he could receive help and support from facility expert, during the analysis.

Benefits

- Provide a user friendly environment (most of our users are not expert neither in data treatment, neither in IT and some have no home IT support).
- Accelerate the analysis process, ease collaboration during analysis.
- Solve the problem of transport of experimental data to home labs.
- Move the work from 'software installation' to 'scientific analysis'.
- Authorize the preservation of the full workflow.

Status

- PaNDaaS was not funded
- Coordination meeting between RIs have started to take place (ESRF organisation)
- Work is ongoing mostly with RI budget at the pace allowed by RIs capacity.
- @ILL first users (IN5 instrument) expected for Mid 2017.
- EOSC has the solution?

Contact: data@ill.eu
Portal: <https://data.ill.eu>
Policy: <https://www.ill.eu/DataPolicy>
PaNData Collaboration: <http://pan-data.eu>



research reactor FRM II at Garching near Munich

scientific use through Heinz Maier-Leibnitz Zentrum (MLZ)



== Computing at MLZ ==

- Data analysis:

Heavy investment, group of 6 working on software for

- reflectometry/GISAS simulation and fitting

(project BornAgain, partly supported through SINE2020/WP10)

- TOF data reduction (using Mantid)

- QENS data analysis (integration with Mantid to be investigated)

- data reduction for materials diffractometer

- data reduction for single-crystal diffraction (NSXTool, collaboration with ILL)

In the future, we will also develop software for the ESS (part of the German in-kind contribution)

- Instrument control:

Since instruments were built by many different institutes, conversion to unified electronics and software is still ongoing. Standard platform is now NICOS on top of TACO/TANGO.

- Data archival:

All data are stored at the instruments, copied to central servers, and archived externally (Leibniz Rechenzentrum).

- Data portal:

Universal data portal offered by Library of Technische

Universität München. With forthcoming high data flow instruments, we need to reconsider

domain-specific solutions from ISIS or ILL.

A decorative graphic in the top right corner consisting of numerous thin, overlapping lines in various colors (yellow, green, blue, purple, pink) that fan out from a central point towards the right edge of the slide.

== Big data? ==

- So far, no instrument in event mode.
 - Tomography instrument is producing several TB/experiment; users go home with data on hard disk.
- Domain-specific software, not under responsibility of central computing group.
- In 2017, commissioning of DNS TOF mode, up to 30 GB/day.
 - In 2018, commissioning of TOPAS, up to 100 GB/day.
 - Then, commissioning of PowTex, at least similar data rate.

Therefore, increasing interest to adopt data flow solutions developed at other institutes.