

Icat@ill In 5 min



A bit of history

- 2009 start of the ILL ICAT installation and first meeting on the DP.
- Development of the ILL web interface: <u>http://icatprod.ill.fr:8585/icat</u>
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- Dec 2011, publication of the ILL Data Policy http://www.ill.eu/users/ill-data-policy/

Only now we can start working efficiently: The project has moved from an IT project to an ILL project.



Our technical difficulties

- Lack of systematic link between the raw data and proposals and finally users.
- Too many data formats => Ingestion is a nightmare.
- What are the useful experimental parameters?
- Ontology, diversity of naming conventions.
- Doing things urgently => bad coding strategy (use of SQL statements instead of developing Web Services)



Today

- Scientists are on board (DPP).
- 19th of April, test of 'fake' user authentication on IC workstation.
- Installation of ICAT 4.0 and TopCat.
- ICAT 4.0/1 vs ICAT 3.3 for the rollout?
- Ingestion production planned for September (DP official introduction)
- The ILL DP might require some works on the access right management.

A global picture



Increase scientific data value Long term data curation

1

Draw up a clear Data Policy



IT security enforcing data policy



Adding necessary metadata for interpretation later on

Data Set definition

Collect useful parameters

Link to proposal system

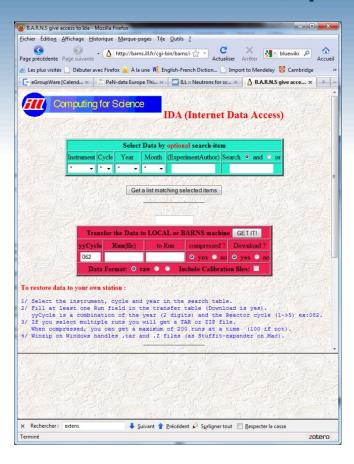
File format standardization when possible

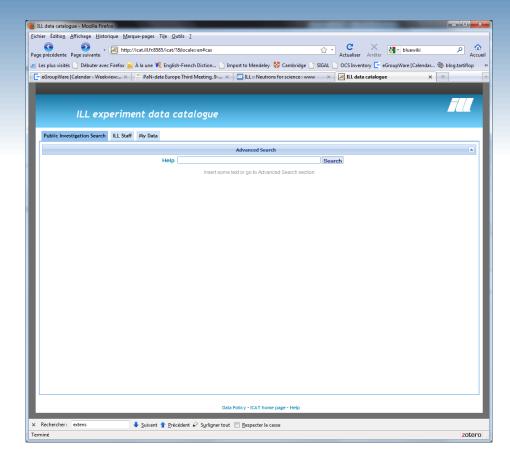
ICAT new data catalogue (search by metadata)



ICAT a successor to IDA

http://icat.ill.fr:8585/icat/







iCat@ill status

- Ongoing
 - Migration to iCat V4.0
 - Web interface : the ILL one of TopCat ?
 - We are currently installing topcat for testing
- To be done
 - Seal the link between proposals and data files
 - Implement Access Right management according to the Data Policy (workflow, interfaces, ...)
 - Validate the ingestion process
 - DOI implementation
 - Rollout and communication

Technical contact: Holger Gebhard <u>gebhard@ill.eu</u> or Me



User Authentication

- The problem: currently all applications have their own local repository
- End of February Merge of the different accounts (1st step accounts from VC)
- Next: typo, forge, wifi, storage, computers
- Evaluation of the EU wide authentication

Project contact: Fabien Pinet pinet@ill.eu or Me



Storage

- Security: ACLs implementation and access protocols NFSv4, CIFS, ...
- Adding more informations (images, log, E-Logbook ...) – Folder structure change?
- Facing the volume groth change in the infrastructure solution (FS compression, deduplication, decrease the cost per TB, ...)

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Projects on the EU side.

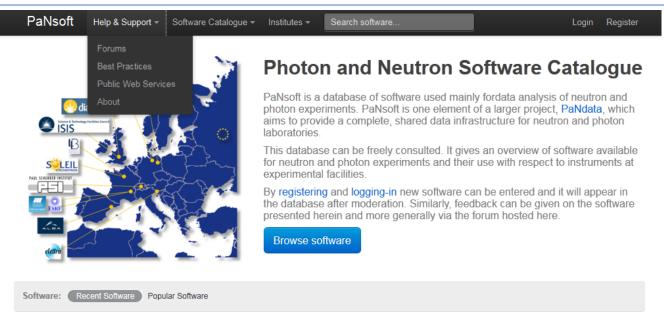
PaNdata-Europe, PaNdata-ODI, CRISP, NMI3, PaNgea, ...

- EU Common Authentication
- Evolution of iCat (data mining, cross repository search, link with the publications, LT Preservation – OAIS)
- Software analysis catalogue PaNSoft
- High-speed Data Recording

• ...



PaNsoft



Recent Software

NAMD

NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems.

PORE3D

large software suite for filtering, segmentation and quantitative analysis of 3D images (CT, MRI, CLSM, ...).

Ominc

Logiciel d'acquisition des spectres infrarouge. Ce logiciel permet aussi un de créer des cartographies

IMOD

IMOD is a set of image processing, modeling and display programs used for tomographic reconstruction and for 3D reconstruction of EM serial sections and optical sections.

IVE+PRIISM

collection of tools for processing, analyzing, and visualizing multidimensional imagery with a focus on 3D wide-field optical microscopy and EM tomography





Our expectation from that group

- Help to communicate
 - With the other ILL scientists
 - With the users
- Give your feedback
- Validate Test Bring your scientific expertise
- Bring the real users' needs Propose ideas
- Work togheter closer than in the past
- Your support