

# PaNdata Software Catalogue

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## Objective 6 – Software

To determine how to develop, deploy, operate and evaluate a common registry of data analysis software and, where appropriate, the necessary format converters, so that data from different sources can, in the future, be treated with a variety of data analysis software.

*... More ‘passionately/ambitiously’ ...*

Data analysis (software) is a key link in the chain of events that transforms original ideas into conclusive scientific output. The approach of this WP is therefore to help define a **common software resource** that will:

- simplify and streamline for facility users the conversion of raw data into high quality scientific data for publication,
- accelerate the deployment and use of new data analysis methods which will open doors to new science across the facilities and the user community,
- enhance and optimise the scientific output of the facilities i.e. better value for money.

# D6.1: List of software (~250)

Name of software	Entered by	Affiliation	URL homepage	Brief description	Field of application	N/M/X/P
A2Tool	A. Rothkirch	DESY		Tiny Tool for visualization and batch processing of image diffraction data - allows batch processing for simple azimuthal/circular integration of 2d data	pre processing of 2d data	X-ray (and neutron ?)
Aclimax	Robert McGreevy	ISIS	<a href="http://www.isis.rl.ac.uk/molecularSpectroscopy/tosca/">http://www.isis.rl.ac.uk/molecularSpectroscopy/tosca/</a>	Inelastic neutron spectroscopy simulation software based upon existing vibration data designed to produce a spectrum that can be compared with experimental data.	Inelastic neutron spectroscopy	neutron
ADXV	BAC & PICCA	Soleil	<a href="http://www.scripps.edu/~arvai/adxv.html">http://www.scripps.edu/~arvai/adxv.html</a>	Data visualisation/model building/analysis.	Protein Crystallography	X-Ray
AMORE	BAC & PICCA	Soleil	<a href="http://mem.ibs.fr/JORGE/index.html">http://mem.ibs.fr/JORGE/index.html</a>	Processing. Molecular Replacement.	Protein Crystallography	X-Ray
anatric	Mark Koennecke	PSI		Integration of four circle area detector data	Single crystal	neutron
APBS	BAC & PICCA	Soleil	<a href="http://www.poissonboltzmann.org/apbs/">http://www.poissonboltzmann.org/apbs/</a>	Adaptive Poisson-Boltzmann Solver	Protein Crystallography	X-Ray
Ariel	Robert McGreevy	ISIS	<a href="http://www.isis.rl.ac.uk/disordered/gem/Software/Ariel3.1.release.htm">www.isis.rl.ac.uk/disordered/gem/Software/Ariel3.1.release.htm</a>	Data reduction/visualisation software package for handling data collected on the GEM, OSIRIS and HRPD powder diffraction instruments at ISIS	Crystallography	neutron
ARPWARP	BAC & PICCA	Soleil	<a href="http://www.embl-hamburg.de/ARP/">http://www.embl-hamburg.de/ARP/</a>	Automatique tracing and phase improvement	Protein Crystallography	X-Ray
ASTEXVIEWER	BAC & PICCA	Soleil	<a href="http://www.astex-therapeutics.com/AstexViewer/index.php">http://www.astex-therapeutics.com/AstexViewer/index.php</a>	Data visualisation/model building/analysis.	Protein Crystallography	X-Ray
<i>Athena/Artemis/Hephaestus/Atoms</i>	A. Rothkirch	DESY	<a href="http://cars9.uchicago.edu/~ravel/software/">http://cars9.uchicago.edu/~ravel/software/</a>			
Beamline-B1-macros	A. Rothkirch	DESY	<a href="https://github.com/uvainio/Beamline-B1-macros">https://github.com/uvainio/Beamline-B1-macros</a>	Processes the Pilatus 1M data coming from beamline B1 at DORIS III, using the information from header-files, specific to the beamline. Produces SAXS data integrated into 1D in absolute units and a matching q-range and error.	SAXS	X-ray
BEST	BAC & PICCA	Soleil	<a href="http://www.embl-hamburg.de/BEST/">http://www.embl-hamburg.de/BEST/</a>	Strategy calculation	Protein Crystallography	X-Ray
<i>bkchem</i>	A. Rothkirch	DESY	<a href="http://bkchem.zirael.org/">http://bkchem.zirael.org/</a>	chemical drawing program		
BNP	BAC & PICCA	Soleil	<a href="http://www.hwi.buffalo.edu/BnP/">http://www.hwi.buffalo.edu/BnP/</a>	Processing. Ab initio structure solution and phasing.	Protein Crystallography	X-Ray
BOBSCRIPT	BAC & PICCA	Soleil	<a href="http://www.csb.yale.edu/userguides/graphics/bobscript/bobscript.html">http://www.csb.yale.edu/userguides/graphics/bobscript/bobscript.html</a>	Ray stracing/Representation.	Protein Crystallography	X-Ray

### *Observe (i.e. overview)*

- Large volume of (often legacy, single-developer) software
- Diversity of software
- Diversity of data formats (WP5)
- No obvious author/owner in many cases
- Lack of (often technical) information i.e. Missing metadata
- Limited use of version control
- Limited use of licenses

### *Conclude*

- Considerable challenge to harness and manage this data (short term)
- Rationalise the volume of software (ranking)
- Encourage best practices for software development (software policy WP2)
- Encourage use of software forge and link to catalogue (longer term)

given volume of software and quality/completeness of information ensure that a functional catalogue could be created to allow sharing of existing software

→ *proto-type catalogue*

(concentrate on the catalogue, reflect upon link to and integration with repository and software forge)

**Database Model** : Information collected on each item of software, that is the set of **metadata**. → Minimal set of metadata, managing multiple entries, formatting this data, structuring links between data

The types of **users** that are likely to be concerned by the DB and the roles they will play

→ In particular contributors, authors and contact people

The **web interface** to the DB and the information and function that this will include

→ Clear presentation of software, scheme for rating software i.e. Identifying the most popular and useful codes (→ common, key software), best practices...

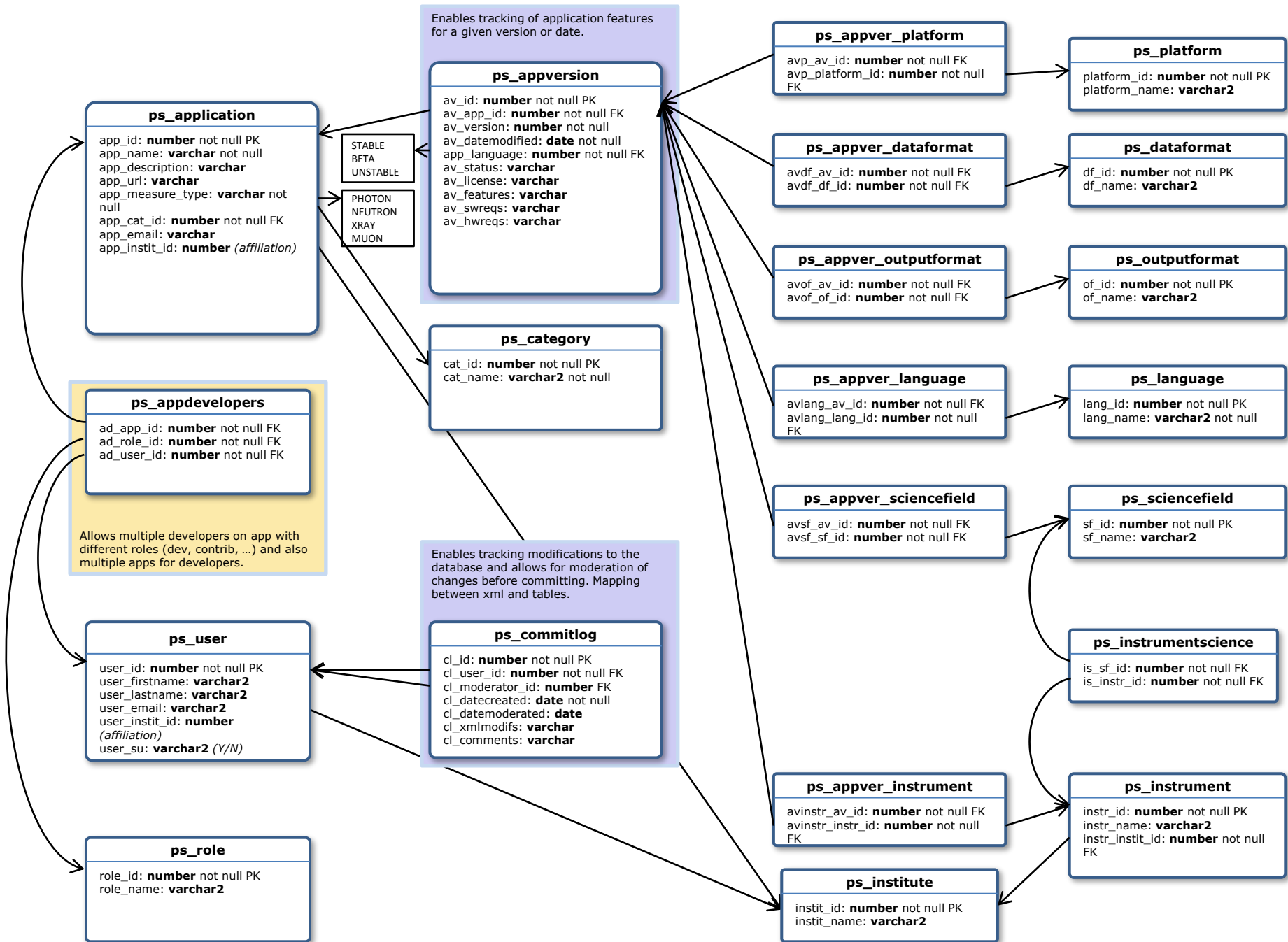
The **Web Services** for using the information outside the portal

→ iCat integration, Information System of facilities ...

# structuring the metadata

- restricting input ('controlled vocabulary')
- efficient searching
- integration with data catalogue (ICAT)

Categories for software and instruments				
instruments	ILL	ISIS	PSI	LLB
diffraction	D1a, D2b, D3, D4, D7, D19, D20, D1b, D15, D23, LADI, VIVALDI, SALSA	Gem, Engin-X, Hrpd, Nimrod, Osiris, Pearl, Polaris, Rotax, Sandals, SXD, Wish, Ines	DMC, HRPT, MORPHEUS, POLDI, TRICS	3T-2, G4-1, G4-2, G6-1, 5C-1, 5C2, 6T-2, 7C-2, 6T-1
spectroscopy	IN1, IN4, IN5, IN6, IN8, IN10, IN12, IN13, IN14, IN15, IN16, IN20, IN22, BRISP	Iris, Maps, Mari, Merlin, TOSCA, Vesuvio, Let, Osiris	FOCUS, MARS, RITA-II, TASP	1T-1, 2T-1, 4F-2, G4-3, Mibemol, Muses
large scale structures	D11, D16, D17, D22, FIGARO, ADAM, SUPERADAM	Crisp, Inter, Offspec, Polref, Surf, Loq, Sans2d, Nimrod, Sandals	AMOR, SANS-I, SANS-II	Pace, Paxy, Paxe, TPA, Papyrus, Eros, Prism
muons		Argus, Emu, Hifi, MuSR	DOLLY, GPD, GPS, LEM, ALC, LTF	
nuclear and particle physics	PF1, PF2, PN3-GAMS, CRYOEDM, GRANIT			
imaging			ICON, NEUTRA	
other	S18 (interferometer)			





The screenshot shows a web browser window displaying the PaNsoft website. The browser's address bar shows 'http://pandata.ill.fr/'. The website's navigation bar includes 'PaNsoft', 'Help & Support', 'Software Catalogue', 'Institutes', 'Search software', 'Login', and 'Register'. The main content area features a map of Europe with various neutron and photon facilities marked, including Diamond, ISIS, ESRF, and ILL. To the right of the map is the title 'Photon and Neutron Software Catalogue' and a brief description of the database. Below the map is a 'Browse software' button. A tabbed interface shows 'Recent Software' and 'Popular Software'. Under 'Recent Software', several software entries are listed: NAMD, PORE3D, Omnic, IMOD, and IVE+PRIISM, each with a short description of its function.

**Photon and Neutron Software Catalogue**

PaNsoft is a database of software used mainly for data analysis of neutron and photon experiments. PaNsoft is one element of a larger project, PaNdata, which aims to provide a complete, shared data infrastructure for neutron and photon laboratories.

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. Similarly, feedback can be given on the software presented herein and more generally via the forum hosted here.

[Browse software](#)

Software: [Recent Software](#) [Popular Software](#)

### 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, MR, CLSM, ...)

**Omnic**  
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

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[Browse software](#)

Software: [Recent Software](#) [Popular Software](#)

### 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

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#### 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

## Search Results

### Filter Results

#### Institutes

ALBA Synchrotron Light Facility  
 DESY (Deutsches Elektronen-Synchrotron)  
 Diamond Light Source  
 ELETTRA Synchrotron Light Facility  
 European Synchrotron Radiation Facility  
 Helmholtz-Zentrum Berlin  
**Institut Laue-Langevin** ✖  
 ISIS neutron source  
 Laboratoire Léon Brillouin  
 Paul Scherrer Institut  
 Soleil Synchrotron

#### Categories

Your search for molecular returned 2 results. Use the options on the left to filter the results.

#### 1. **NAMD**

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

#### 2. **nMoldyn**

nMOLDYN is an interactive analysis program for Molecular Dynamics simulations. It is especially designed for the computation and decomposition of neutron scattering spectra, but also computes other quantities.

← Previous 1 2 3 4 5 Next →

PaNsoft Help & Support Software Catalogue Institutes Search software Login Register

Search **Neutron Software Catalogue**

Submit your software to the catalogue

Search Catalogue

Search over 250 applications. To get started please enter a search term into the box

Software Catalogue Browse

## Category

- Instrument Simulation
- Protein Crystallography
- Diffraction
- Sample Simulations
- Spectroscopy
- Large Scale Structures
- Muons
- Imaging
- Absorption

Displaying 1 items of software



### 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.

Categories [Imaging](#)

Current Version 4.1

License Free



### IVE+PRIISM

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

Categories [Imaging](#)

Current Version 4.2

License Free



### LABSPEC

Logiciel d'acquisition de données Raman et Fluorescences

Categories [Imaging](#)

Current Version Unknown

License Free



### Ormisc

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

Categories [Imaging](#)

## nMoldyn

nMOLDYN is an interactive analysis program for Molecular Dynamics simulations. It is especially designed for the computation and decomposition of neutron scattering spectra, but also computes other quantities.



Website	<a href="https://forge.epn-campus.eu/projects/show/nmoldyn/">https://forge.epn-campus.eu/projects/show/nmoldyn/</a>
Current Version	3.0.9
License	Unknown
Categories	<a href="#">Diffraction</a>
Institute	<a href="#">Institut Laue-Langevin</a>
Institute Instrument	<a href="#">D11</a>
Authors	<a href="#">Gerald Kneller</a>
Contributors	<a href="#">Gerald Kneller</a>

Select a version

**3.0.9 (current)**

Rating

★ ★ ★ ☆ ☆

### Specifications for version 3.0.9

Version	3.0.9
Software Requirements	-
Hardware Requirements	Python, NumPy, Matplotlib, PyRO, ScientificPython, MMTK
Platforms	<a href="#">Windows</a>
	<a href="#">Mac OS</a>
	<a href="#">Linux</a>
Languages	<a href="#">Python</a>
Input Formats	
Output Formats	

### Comments

To leave a comment you must be registered user. If you're registered, please login.

## Web Services

PaNdata's API exposes much of the PaNdata infrastructure via a standardised programmatic interface.

### Details

[Overview](#)  
[Authentication](#)  
[ICAT Integration](#)

### Methods

[Search software](#)  
[Get details for a piece of software](#)  
[Get institute details](#)  
[Get all institutes](#)

### Technology Overview

The PaNsoft API is a RESTful API based on HTTP requests and XML or JSON responses. If you're familiar with the APIs of Twitter, Amazon's S3, del.icio.us, or a host of other web services, you'll feel right at home.

### End points

The API is accessed by making HTTP requests to an endpoint URL, in which GET or POST variables contain information about what you wish to access. Every endpoint is accessible via standard HTTP (port 80) and SSL-enabled HTTPS (port 443).

The default HTTP endpoint is:

```
http://api.pansoft.eu
```

The default HTTPS endpoint is:

```
https://api.pansoft.eu
```

### Response Formats

Responses are either XML (the default) or JSON. Response formats are specified by supplying an extension to the API call. For example, to specify a JSON call to get all institutes, the URL is:

```
http://api.pansoft.eu/institutes.json
```

and to specify an XML response, the URL is:

```
http://api.pansoft.eu/institutes.xml
```

### Examples

Here is a quick example of how to get software by an institute. In this example we're getting all of the software related to Institut Laue-Langevin returned in JSON

API call

```
curl -v -H "Content-Type:application/json" -H "Accept:application/json"  
http://api.pansoft.com/institutes/institut-laue-langevin/software.json
```

API Response

```
< HTTP/1.1 201 Created  
< Connection: close  
< Date: Fri, 10 Sep 2010 14:58:49 GMT  
< Location: http://api.pansoft.com/institutes/institut-laue-langevin/software.json
```

### Questions? Feedback?

Have you run into difficulties or a method just doesn't seem to work right? Check out our API Support options [here](#) and we'll be happy to assist you.

## Achievements :

- Graphical Design
- Database structure
- Display interfaces
- Software submission
- Registration
- Search Engine
- Basic web services
- ...

The screenshot shows the 'Submit your software to the catalogue' page on the Pansoft website. The page has a dark header with the Pansoft logo, navigation links for 'Help & Support', 'Software Catalogue', and 'Institutes', a search bar, and 'Login' and 'Register' buttons. Below the header, a blue banner says 'Thank you for choosing to add your software to the catalogue.' The main content area is titled 'Submit Software to Catalogue' and contains a 'Version Details' section. This section includes a green message box: 'Now we would like to know about the version details of your software.' Below this are several form fields: 'Version' (text input), 'Platforms' (dropdown menu with 'Mac OS' selected), 'Output Formats' (dropdown menu with 'LL TAS Data Format' selected), 'Input Formats' (dropdown menu with 'LL TAS Data Format' selected), 'Languages' (dropdown menu with 'Java' selected), 'Hardware Requirements' (text area), and 'Software Requirements' (text area). Each field has a corresponding question to its right, such as 'Please enter the current version of the software...' and 'Which platforms does your software run on?'.

## To be refined :

- Management interfaces (licenses, Instruments, ...)
  - Management of Comments and Rating
  - Finalize the infrastructure
  - Clean up the information
  - Name ?
- 
- Public rollout of the prototype
- Mid April 2012**

**PaNsoft** Help & Support Software Catalogue Institutes Search software... Login Register

## Web Services

PaNData's API exposes much of the PaNData infrastructure via a standardized programmatic interface.

### ICAT Integration

ICAT is a database (with supporting software) that provides an interface to Large Facility experimental data and will provide a mechanism to link all aspects of the research chain from proposal through to publication.

**Details**

- Overview
- Authentication
- ICAT Integration

**Methods**

- Search software
- Get details for a piece of software
- Get institute details
- Get all institutes

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Name	Description	Author	Download File
ICAT Integration	ICAT Integration	ICAT Integration	ICAT Integration
ICAT Integration	ICAT Integration	ICAT Integration	ICAT Integration
ICAT Integration	ICAT Integration	ICAT Integration	ICAT Integration
ICAT Integration	ICAT Integration	ICAT Integration	ICAT Integration



Not yet done, planned for the summer

- Full set of Web Services
- TopCat integration
- Umbrella integration

In a longer term :

- Persistent Identifiers for SW
- Forum integration ?
- Link with a SW forge

Please feedback