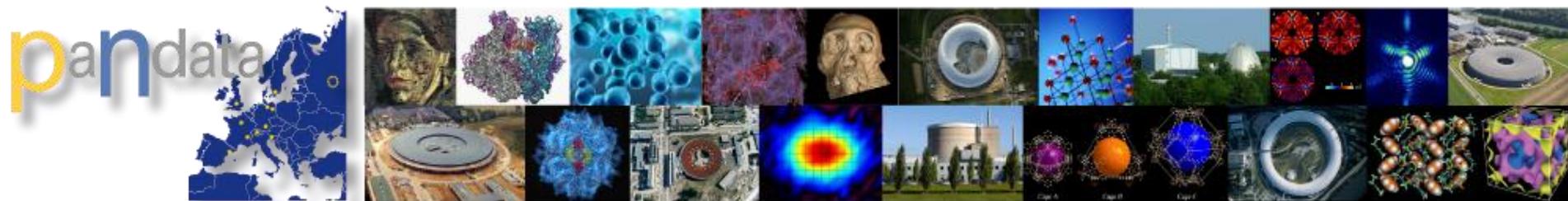


PANData Software Catalogue

Jamie Hall
Developer
IT Services, Institut Laue-Langevin
30th January 2013. CERN

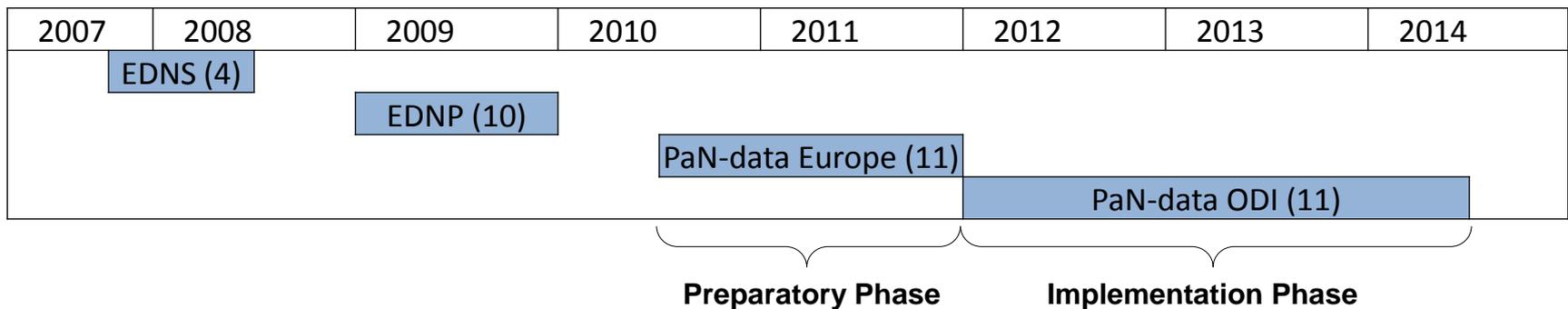


PHOTON AND NEUTRON DATA INFRASTRUCTURE

pandata

Established 2007 with 4 facilities

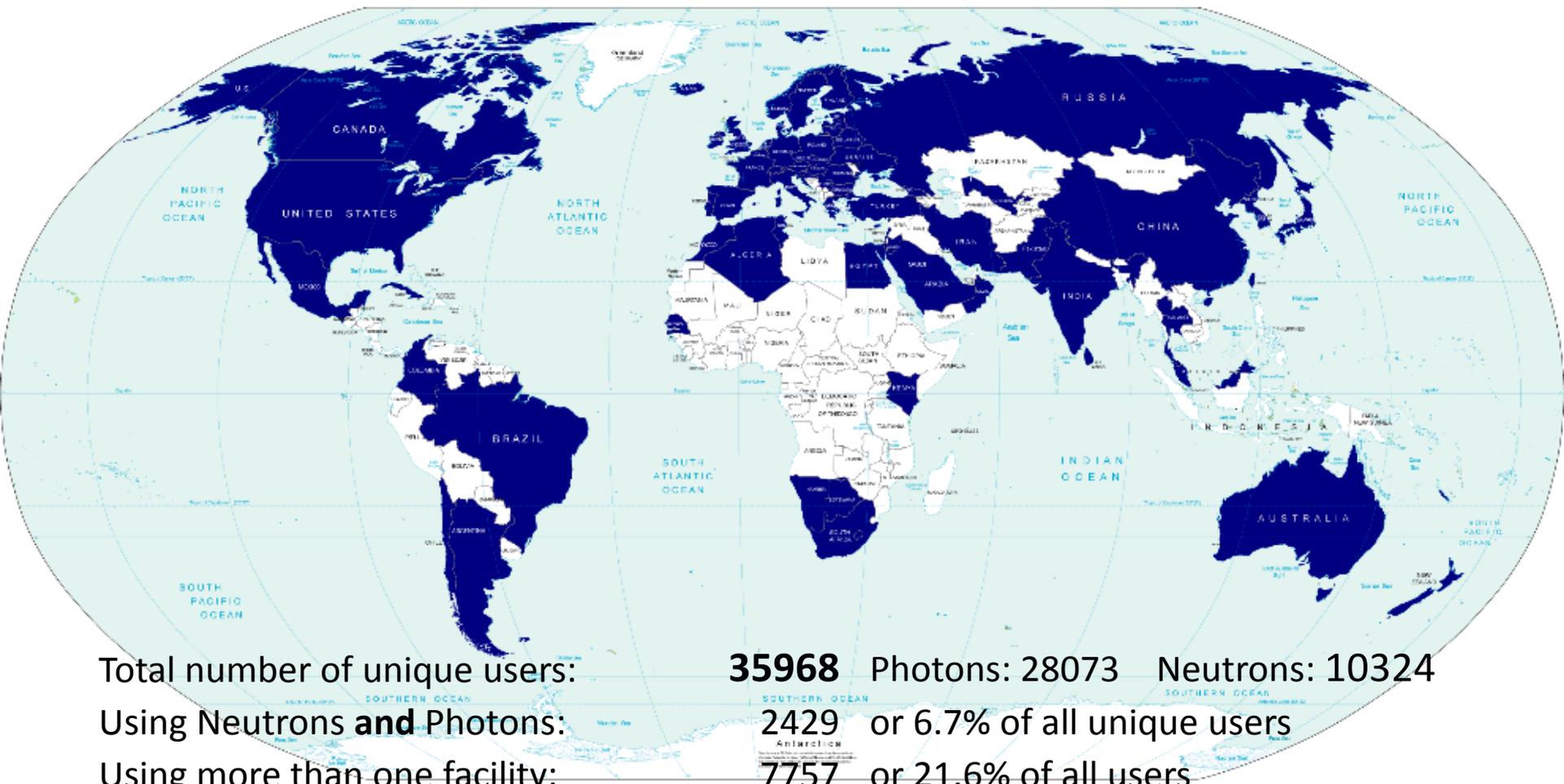
Expanded since to 13 facilities



PaNdata is a joint effort of currently 13 major world class European x-ray and neutron research facilities providing experimental opportunities to a broad range of scientific communities world wide.

PaNdata aims to create a fully integrated pan-European, information infrastructure supporting the scientific process.





Total number of unique users:	35968	Photons: 28073	Neutrons: 10324
Using Neutrons and Photons:	2429	or 6.7% of all unique users	
Using more than one facility:	7757	or 21.6% of all users	

 PaNdata users

- Harmonise authentication and authorisation
- Standardise data formats and annotation of data
- Allow transparent and secure remote access to data
- Establish sustainable and compatible distributed data catalogues (cross search engine)
- Provide compatible data analysis software
- Promote data policies in laboratories
- The Infra should cover the whole continuum (from proposal to publication)
- Allow long term preservation of data

THE SOFTWARE CATALOGUE

PANData Software is a web application which provides users with the necessary tools to find, collaborate and get involved with Photon and Neutron software

 **Please note:** This website is currently in a **BETA** state. It is in the process of heavy development. Certain aspects of the website are likely to change. Furthermore, certain functionalities may not work.

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](#)



RECENT SOFTWARE



NAMD

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



MOLREP

SEARCH FOR SOFTWARE

Looking for a piece of software? Use the search box below to find it.

- Provide scientists with a centralised catalogue of software they can use to solve their problem
- Help users decide on the best software to use to fulfill their needs
- Help developers through the use of versioning, best practices and hierarchical data architecture to publicise their software
- Unique opportunity – de-facto place to go for Photon and Neutron Software
- Aggregate and share knowledge

Lots of software and we don't know their state:

- Version
- Authors and contributors
- License
- Data formats
- Hardware requirements
- Software requirements
- Attributed to an institute
- Website
- Languages
- And much more...

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Web Services

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

- DETAILS
- [Overview](#)
- [ICAT Integration](#)

Technology Overview

The PaNdata API is a RESTful API based on HTTP requests and JSON (JSONP is also supported) 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. The current version of the API is **V1**.

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://software.pandata.eu/api/v1
```

The default HTTPS endpoint is:

```
https://software.pandata.eu/api/v1
```

Response Formats

All responses are returned in JSON. For example, to specify a JSON call to get all institutes, the URL is:

```
https://software.pandata.eu/api/v1/institutes.json
```

We also support JSONP.

Questions? Feedback?

Have you run into difficulties or a method just doesn't seem to work right? Post a message in our [support forum](#)



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Search 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

Data Analysis
 Instrument Simulation
 Sample simulation

Data Formats

ASCII
 FullProf
 HDF5
 IDL
 ILL TAS Data Format
 Instrument Raw Data
 NetCDF
 NeXus
 PDB
 RAW
 RAW
 TIFF
 User Generated
 XDATCAR

Your search for returned 7 results. Use the options on the left to filter the results.



LAMP (runtime)

Large Array Manipulation Program. General Data Inspection, Reduction and Analysis software framework.



MagDraw

Magnetic Editor Cell Constructor



Materials Studio

Materials Studio is a software suite for atomistic simulations including DFT, force field methods and others.



NAMD

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



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.



Phonon

PHONON is a code to calculate lattice dynamics, mainly using input force constants from ab initio (DFT) codes like VASP. There are many kinds of output including spectroscopic scattering functions.



VASP

VASP is an ab initio simulation package based on DFT



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NAMD

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



Details

Screenshots

Overview

Website <http://www.ks.uiuc.edu/Research/namd/>

Current Version 2.7

License Unknown

Categories [Sample simulation](#)

Beam types

Institute [Institut Laue-Langevin](#)

Users



hall

Maintainer

Contributor

 **Please note:** This website is currently in a **BETA** state. It is in the process of heavy development. Certain aspects of the website are likely to change. Furthermore, certain functionalities may not work.



Institut Laue-Langevin

Grenoble, France

With its international funding and expertise the Institut Laue-Langevin (ILL) offers scientists and industry the world's leading facility in neutron science and technology. From its Grenoble site in the south-east of France the Institute operates the most intense neutron source on earth.



Website <http://www.ill.fr>

Categories [Sample simulation](#)

Software Instruments Users

category ▾



NAMD

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

Categories [Sample simulation](#)

Current Version [2.7](#)

License [-](#)



MagDraw

Magnetic Editor Cell Constructor

Categories [Sample simulation](#)



Please note: This website is currently in a **BETA** state. It is in the process of heavy development. Certain aspects of the website are likely to change. Furthermore, certain functionalities may not work.

Forum

Welcome to the forum. To create a topic you will need to create an account

[Add a new Category](#)

Category	Topics	Posts	Last Post	Actions	
General Discussion General discussion. talk about anything here	0 topic	0 post	30-01-2013 05:00	Edit	Delete
Help & Support Ask questions here about a piece of software or using the web services to receive help and support from other users of the site.	1 topic	1 post	30-01-2013 05:00	Edit	Delete
Development Discuss all topics related to software development and best practices.	0 topic	0 post	30-01-2013 05:00	Edit	Delete
Technology Ask any questions here about any technology you wish to discuss.	0 topic	0 post	30-01-2013 05:00	Edit	Delete
Feedback Got any feedback? Suggestions, ideas and criticism for site is always welcome.	0 topic	0 post	30-01-2013 05:00	Edit	Delete

- Defined as "a software system designed to support interoperable machine-to-machine interaction over a network"
- Communication over the HTTP or the HTTPS protocol
- Return hierarchical data that can be easily read by any programming language
- Expose the data infrastructure via a standardised programmatic interface through a single end point
- Primarily used by developers
- All web services are public
- A user can access data stored in the catalogue through any programming language of their choice
- Return responses in JSON

- PaNdata-ODI Software provides a flexible and scalable search engine which produces realtime and instantaneous results
- Flexible filtering
- Statistics to provide a real insight into:
 - What users are searching for?
 - Which terms are most popular?
 - Which filters are the most interesting?
 - And much more.

- Two options of user authentication
 - Basic authentication
 - Local account with username and password
 - Federated authentication
 - SAML Single Sign On
 - Test implementation with Umbrella
 - Open to other protocols

- Name
- Description
- License
- Contact details
- Categories
- Instruments
- Beam type(s)
- Institute
- Website
- Users
- Screenshots
- Logo
- Versions
 - Version number
 - Software requirements
 - Hardware requirements
 - Platforms
 - Languages
 - Input formats
 - Output formats
- Comments
- Ratings

- Enable users to effortlessly discuss, collaborate and get involved via:
 - Voting and commenting on software
 - Participating in the forums
 - Personal messaging to other users
 - Following PaNdata-ODI Software on twitter
 - Newsletters
 - Individual profiles
 - Taking control of their own software and getting involved in others software



- Integration with ICAT
- Publicity
- Software downloads (mirror)
- Continuous integration
- Apps developed with the PaNdata-ODI software web services (Android, iOS)
- OAuth web services integration
- Statistics
- Continue pushing the NeXus format
- Intelligent software relations
- Long term sustainability
- Linking publications to software
- Persistent Identifiers for software



- How to identify and refer to software persistently ?
 - Sustainability of software's repository ?
 - Sustainability of infrastructure?
 - Ownership ?
 - Contract & licensing ?
 - What to identify? Software, releases, releases per OS, libraries
 - DOI ? Other mechanisms (PURL(Z), ARK, URN, ...)
- Absolute necessity for data preservation and provenance activities.

Questions ?

