Shop-front

Number of Users shared between facilities																
	BER II	BESSY II	DESY	DLS	ELETTRA	ESRF	ILL	ISIS	LLB	SINQ	SLS	SOLEIL	FRM-II	ANKA	neutron	photon	all
BER II	2761	284	152	54	39	319	556	302	156	130	29	38	207	15	814	657	2761
BESSY II	284	7068	487	110	298	810	165	94	72	46	263	260	89	57	475	1601	7068
DESY	152	487	3563	88	121	735	194	91	55	44	155	130	103	43	402	1259	3563
DLS	54	110	88	3494	72	739	213	336	35	18	145	149	20	12	448	989	3494
ELETTRA	39	298	121	72	2731	455	85	43	23	4	66	316	9	20	162	906	2731
ESRF	319	810	735	739	455	10728	886	406	235	92	600	1069	144	80	1389	3463	10728
ILL	556	165	194	213	85	886	4338	741	343	229	69	176	349	10	1577	1280	4338
ISIS	302	94	91	336	43	406	741	2755	120	119	43	52	155	5	958	740	2755
LLB	156	72	55	35	23	235	343	120	1348	34	12	131	92	3	455	375	1348
SINQ	130	46	44	18	4	92	229	119	34	726	96	9	97	0	348	221	726
SLS	29	263	155	145	66	600	69	43	12	96	2424	182	18	18	177	974	2424
SOLEIL	38	260	130	149	316	1069	176	52	131	9	182	3656	14	26	309	1524	3656
FRM-II	207	89	103	20	9	144	349	155	92	97	18	14	1087	5	522	281	1087
ANKA	15	57	43	12	20	80	10	5	3	0	18	26	5	452	29	157	452

Source http://www.pan-data.eu/CountingUsers

Shop-front

Neutron Sources			
Facility	# Users	Users using at least one other Neutron Source	Users using at least one Photon Source
BER II	2761	814 (29.4%)	657 (23.7%)
ILL	4338	1577 (36.3%)	1280 (29.5%)
ISIS	2755	958 (34.7%)	740 (26.8%)
LLB	1348	455 (33.7%)	375 (27.8%)
SINQ	726	348 (47.9%)	221 (30.4%)
FRM-II	1087	522 (48.0%)	281 (25.8%)

Numbers of distinct neutron scattering users for the period Jan 2010 – Jun 2011 per participating facility

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

Using more than one Neutron source: 1983 or **19.2%** of all neutron users

Photon and Neutron Data Infrastructure

History

Who are we ?

The problems

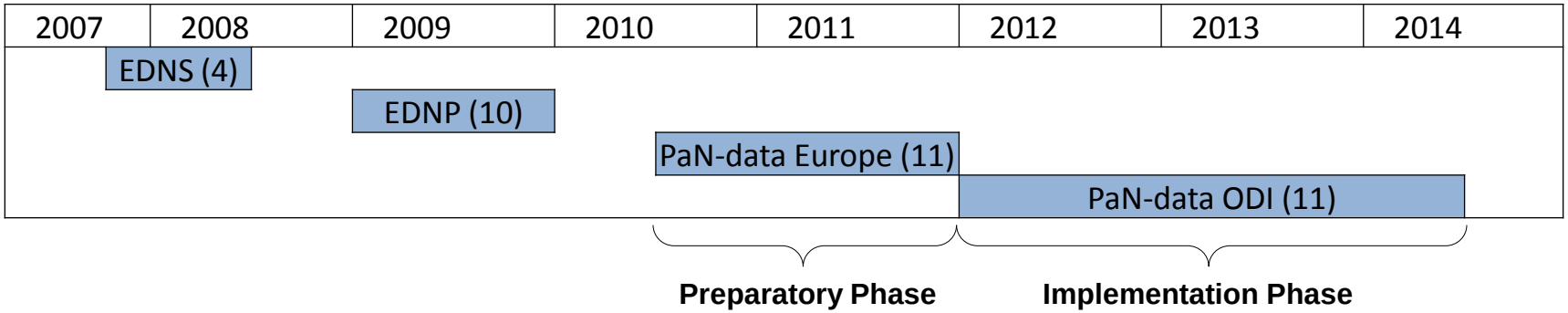
Aims

What has been achieved so far ?

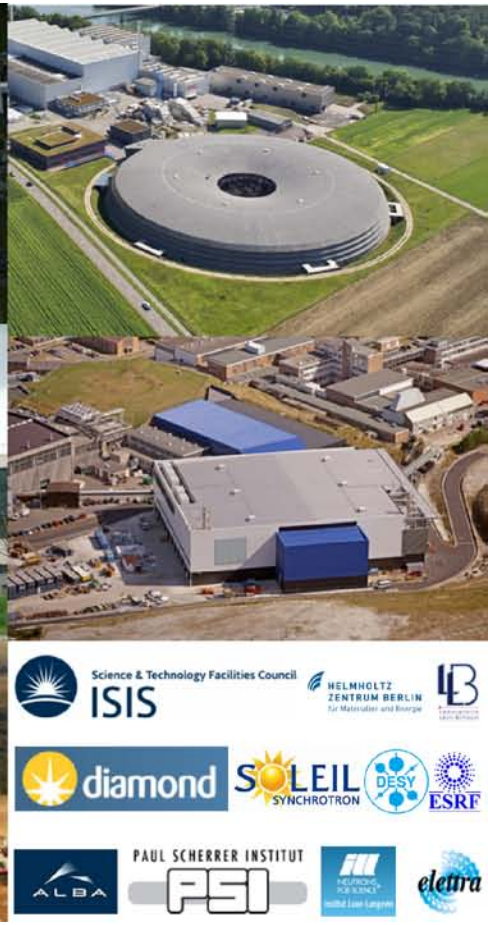
History

Established 2007 with 4 facilities

Expanded since to 11 facilities



Who are we ?



Joining soon : MAX IV ? JCNS ?

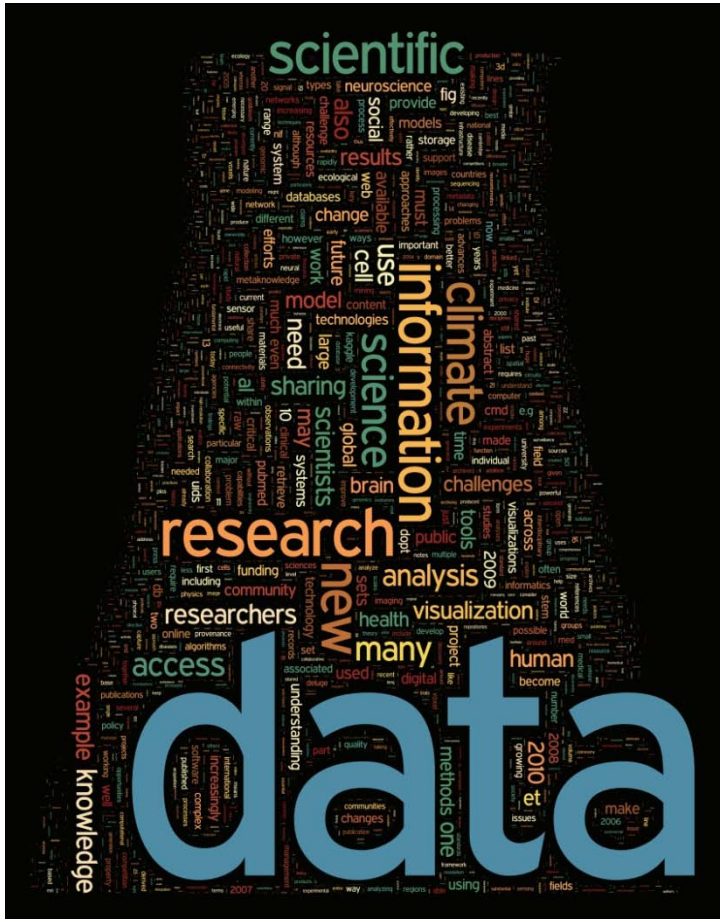
Participants : IT persons and scientists (too few ?)

The problems

1. scientific data is often considered private property
2. open access to scientific data is almost impossible
3. scientific data is not managed professionally
4. barriers to interact with data must be lowered
5. scientists use several facilities for their research
6. the data deluge makes everything worse (mostly X-Ray)

open access to scientific data is almost impossible

- Data is not on-line
- Data is poorly or not described
- No search tools
- No way to identify/cite them
- Authentication/authorisation for scientists is difficult
- Open access is not (yet) well accepted
- Institutions lack infrastructure



scientific data is not managed professionally

ESFRI Position Paper on Digital Repositories:

"Research Infrastructures should guarantee that raw research data are made available through portals and databases."

06/09/2007 – e-IRG ESFRI

nature International weekly journal of science

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

Barriers to interact with data must be lowered
Scientists use several facilities for their research

- Common data file format
- Federated data bases
- Search tools, visualization tools
- EU wide authentication and authorization of scientists
- …

Aims

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

What has been achieved so far where do we stand

Data policy

Authentication

Metadata catalogue

Software catalogue

Data format

Persistent Identifiers for data sets

Data Policy

- We need a clear statement on :
  - Who is the owner
  - If we make them publicly available, how do we protect the Experimental team.
- What do we propose :

1. The facility shall act as a **custodian** for the data.
2. **All raw data will be curated** in a well-defined format with a unique ID.
3. **Metadata** is captured automatically and resides either within the raw data files, and/or in an associated on-line catalogue.
4. **Access to raw data** and the associated metadata obtained from an experiment **is restricted to the experimental team for a maximum period of 3 years**. Thereafter, it will become publicly accessible.
5. The embargo period can be extended on requests.
6. Analysis of openly accessible data must acknowledge the source of the data and cite its unique identifier and any publication linked to the same raw data

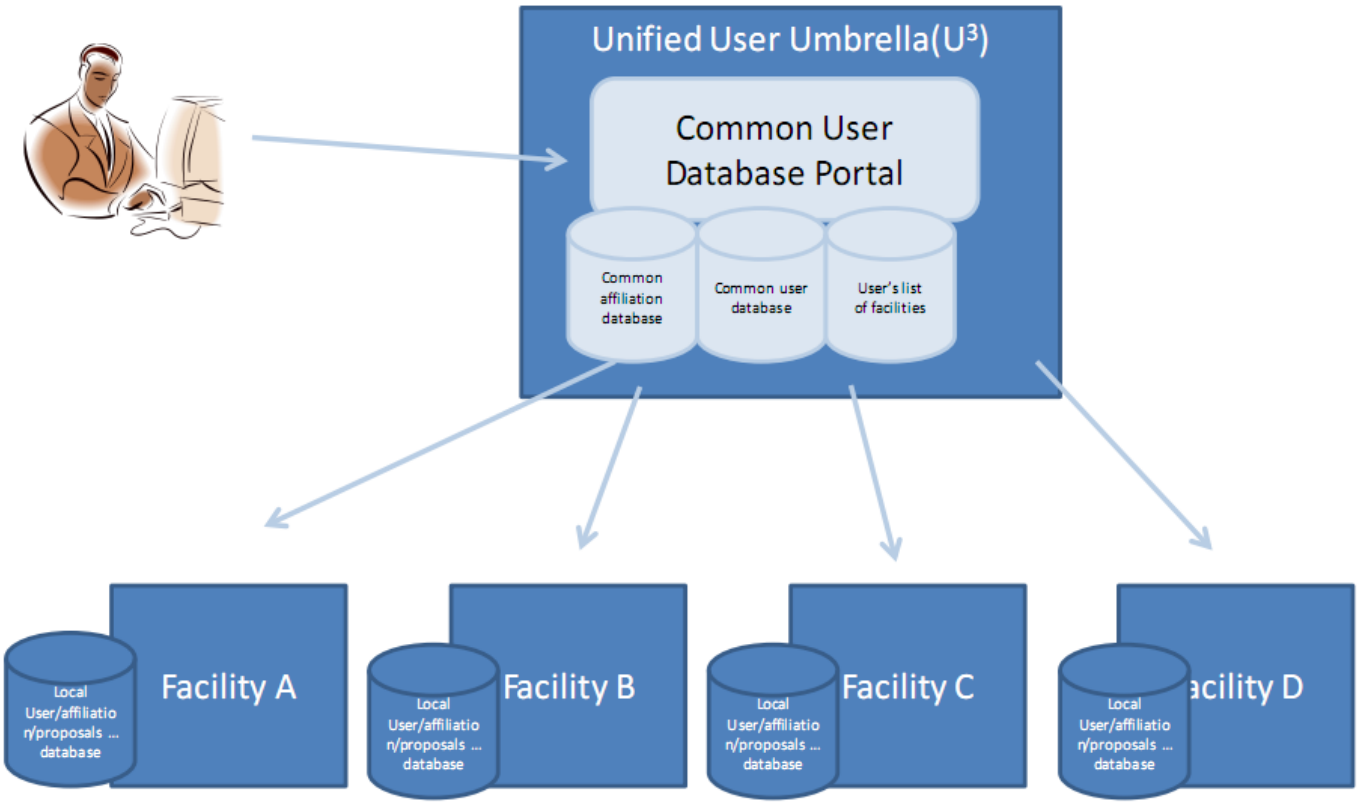
http://www.pan-data.eu/imagesGHD/0/08/PaN-data-D2-1.pdf

Authentication/Identification

- A user should have a single id through the different facilities.
- Federation of Authentication. A user once authenticated by Facility A is automatically identified by Facility B
- Decision on Authorization should remain local to the facility.
- Simple to use : avoid WAYF with long list of IdP, delays for getting certificate, ….
- Should remain persistent when user change its affiliation

Authentication

The user credentials and attributes are managed centrally.



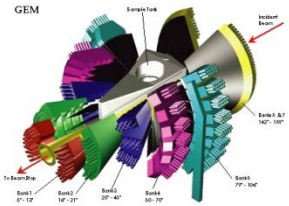
A prototype implementation (based on Shibboleth) is operational

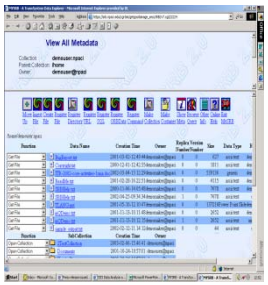
Metadata Catalogue

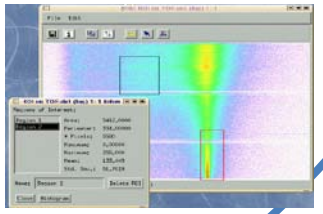
http://www.icatproject.org/

ICAT

Metadata Repository







Proposal

Scientist submits application for beamtime

Approval

Facility committee approves application

Scheduling

Facility registers, trains, and schedules scientist's visit

Experiment

Scientists visits, facility run's experiment

Data cleansing

Raw data filtered and cleansed

Data analysis

Tools for processing made available

Record Publication

Subsequent publication registered with facility

ICAT

- Technically
  - Database schema
  - A set of WebServices i.e You can decide for your own user interface
- Functionalities
  - Allows the aggregation of
    - Experimental parameters
    - Information coming from the proposal system
    - references to datafiles
    - DOIs
  - Implement the security model driven by the data policy
  - Enable cross searching between ICAT instances.

Implemented at ISIS, SNS, Diamond and ILL

Software catalogue

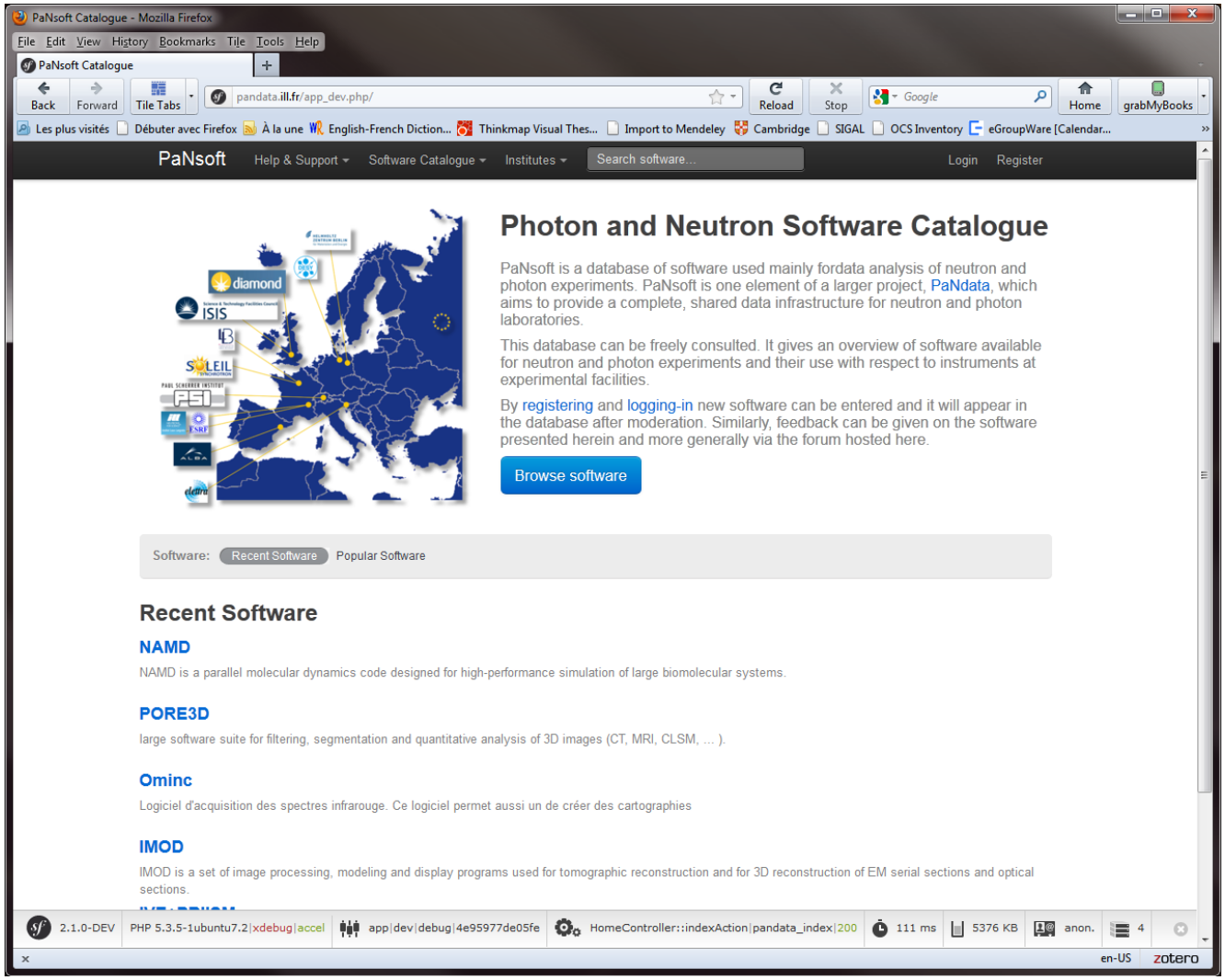
Many software are developed by individuals.

That's great !

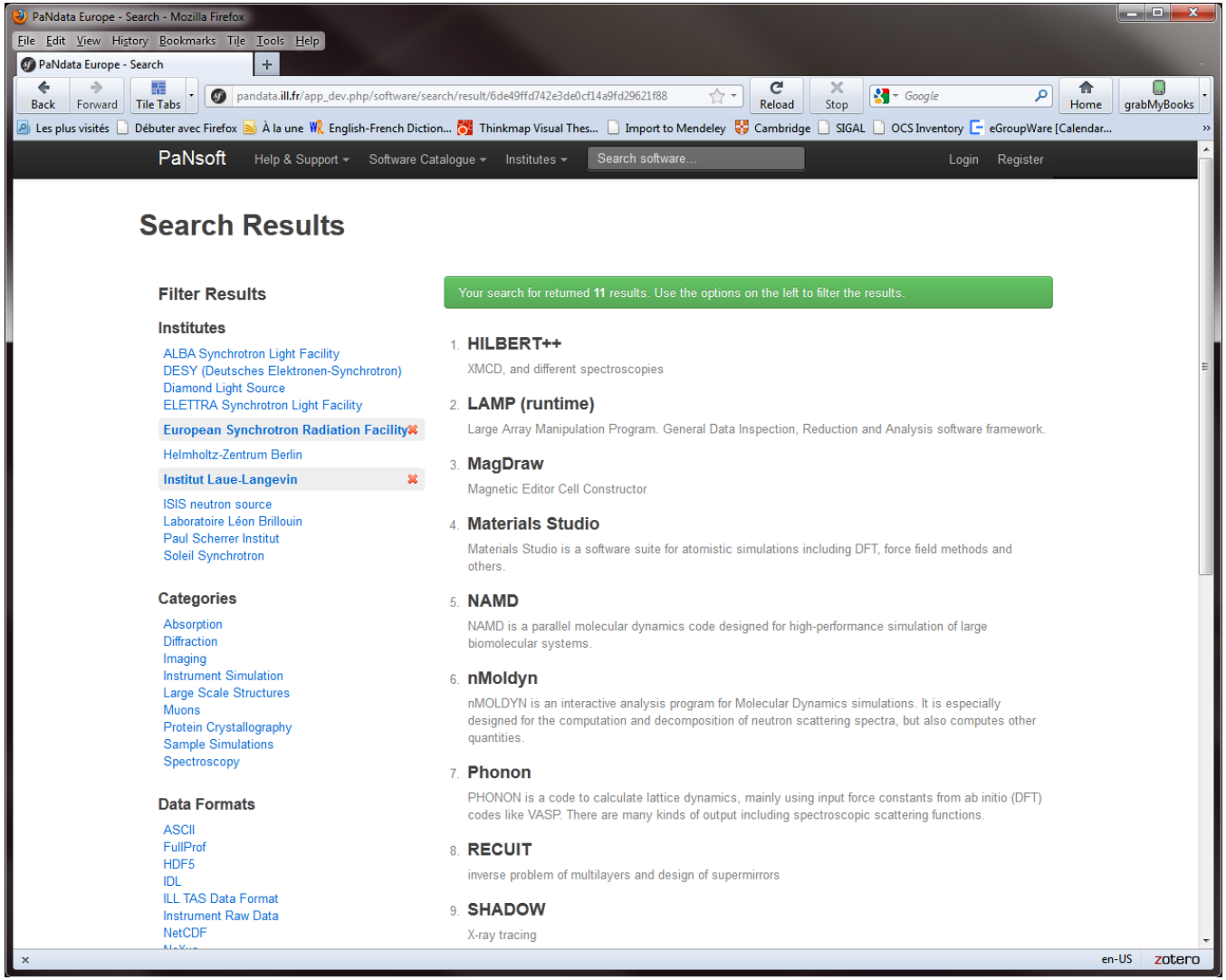
We just want to help to raise up their usability.

- Create / Manage a catalogue of available software (mainly analysis)
- Forster good practice in software development (licences, code versioning, tests, info about support, documentation, …)
- Through Web Services could be integrate in facility portals or ICAT instances

Software catalogue



Software Catalogue



Currently only a prototype.

1st public release Spring 2012

Common data format

- Reduce need for local expertise
- Reduce number of conversion utilities
- Reduce redundant software development
- Increase metadata description – a prerequisite for data archiving/curation
- Increase cooperation in software development
- Increase functionality of generic software
- Create a community standard
- Create critical mass to influence detector manufactures
- Ease cross facility experiments
- …

The PaN-data consortium has decided to adopt

HDF5/Nexus

Slow progress in the deployment

Persistent Identifiers for data sets

DOIs (currently mainly used for journals) for the identification of the raw data sets.

- DOI = 10.5291/ILL-DATA.6-05-579
- http://doi.ill.fr/10.5291/ILL-DATA.6-05-579
- Creator = Investigators/PI
- Title = Proposal Title
- Publisher = Institut Max Von Laue – Paul Langevin
- Date = 3rd December 2010
- Data Format = NXS

Deployment phase at ISIS and ILL

Thanks for you attention

Other projects with related activities :

- DATACITE
- CRISP
- ORCID

Questions ?