

Photon and Neutron Science Interest Group Viewpoint

Brian Matthews

Leader, Data Science and Technology,
Scientific Computing Department

Co-chair of RDA PanSIG



Science & Technology
Facilities Council



- > 50 institutes around the world:
- More X-ray synchrotrons
 - Neutrons
 - Reactors
 - Spallation sources
 - Free-Electron Lasers
 - common users
 - lots of data/computing
 - common needs



Australian Synchrotron

Materials science a major area

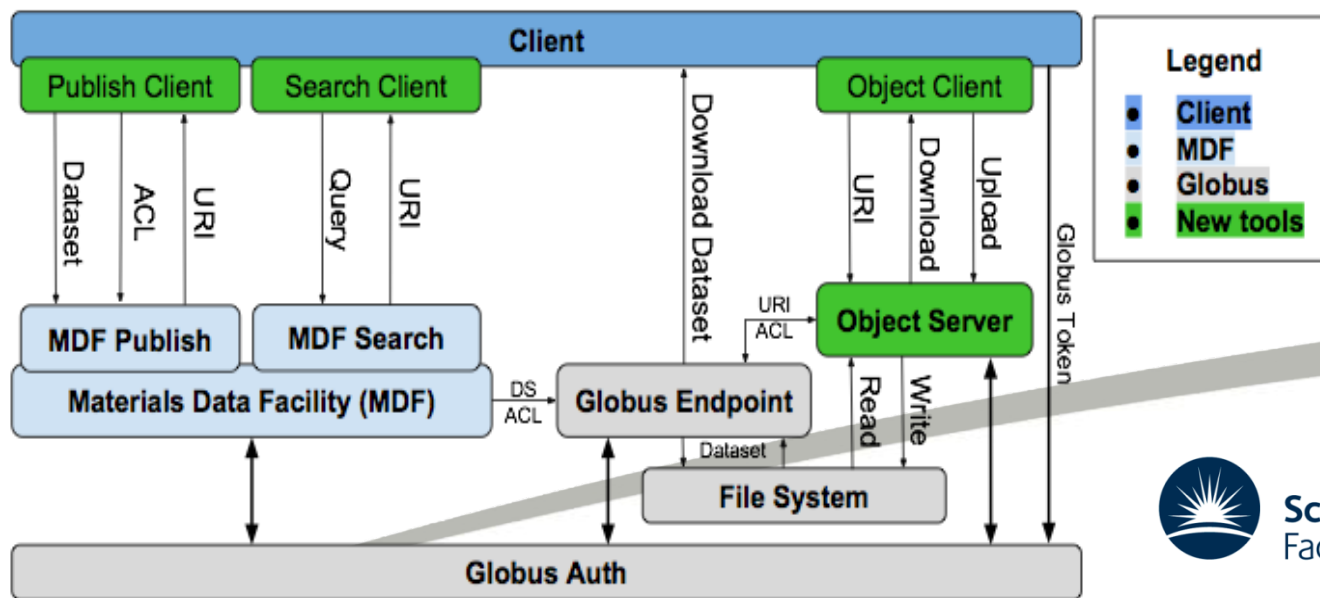
Research data needs of the Photon and Neutron Science community IG (PaNSIG)

- An early interest group
- Chair(s): Amber Boehnlein, Brian Matthews, Frank Schlünzen, Thomas Proffen
- Met regularly at RDA meetings
 - The PaNData Community
 - A good way of keeping the community in contact.
- Workshop on interoperability at ALBA Synchrotron, 3-4 April.
 - Formalise the PaNData Community
 - Explore WG on Data Servers



Catalogue and Share data

- A number of different systems to capture, access and share experimental data
 - E.g. ICAT
 - Metadata catalogue
 - Integrated with Data ingest and downloaders
 - Authorisation and monitoring
 - Used in ISIS, DLS, ESRF, SNS
 - E.g. Materials Data Facility



Topcat

https://data.isis.stfc.ac.uk/#/browse/facility/ISIS/instrument

Science & Technology Facilities Council

Home About Contact Help

Logout (uows/bmm42)

My Data

Browse

ISIS / Instrument

Instrument

Containing...

EVS

GEM

HET

HIFI

Instrument Details

Name: GEM

Description: GEM T

Type: Crystallography

URL: http://www.isis.stfc.ac.uk

Topcat

https://data.isis.stfc.ac.uk/#/browse/facility/ISIS/instrument/28/facilityCycle/71/investigation

Science & Technology Facilities Council

Home About Contact Help

Logout (uows/bmm42)

My Data

Browse

Search

ISIS / GEM / cycle_13_3

Structure of As-Se glasses using neutron diffraction with isotope substitution

Results: 1

Name	Create Time	Modified Time
raw	7.16 GB	2013-11-20 13:40:31

ISIS Home | Privacy Policy | Cookie Policy | About Us

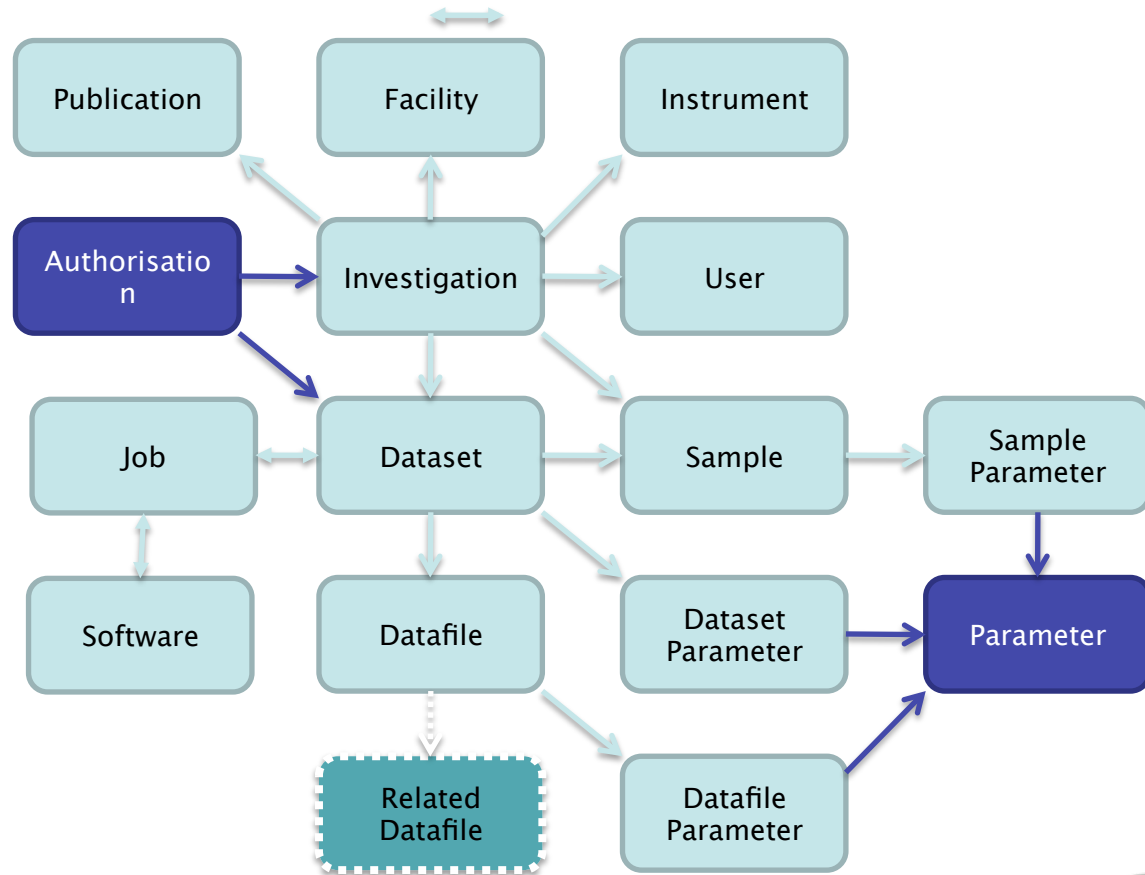
Core Scientific Metadata Model (CSMD)

The Core Metadata model forms the information model for ICAT.

Designed to describe facilities based experiments in Structural Science throughout a facility's scientific workflow.

For use within the repository for organising data

MDF has a similar set of core fields



<http://purl.org/net/CSMD>
<http://icatproject.org/CSMD/>



Science & Technology
Facilities Council

Materials vocab to describe resources

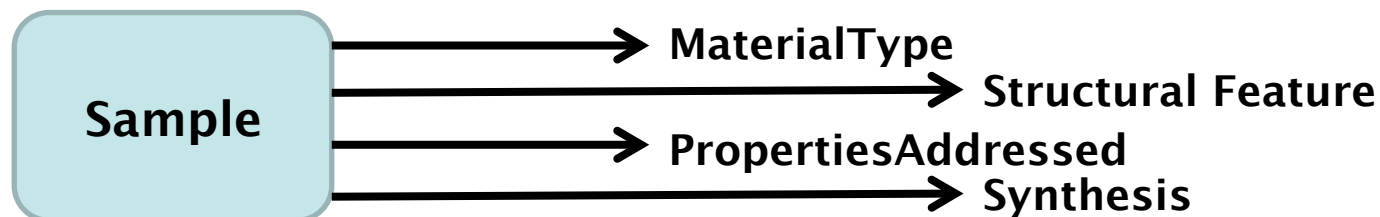
- Major categories
 - Material types
 - Structural features
 - Properties addressed
 - Experimental Characterization methods
 - Computational methods
 - Synthesis and processing
- But what do these categories describe ?



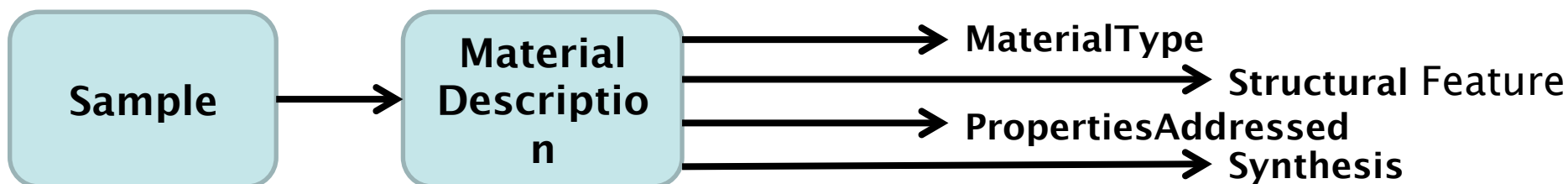
Adding Materials Vocab to CSMD

Metadata Entities

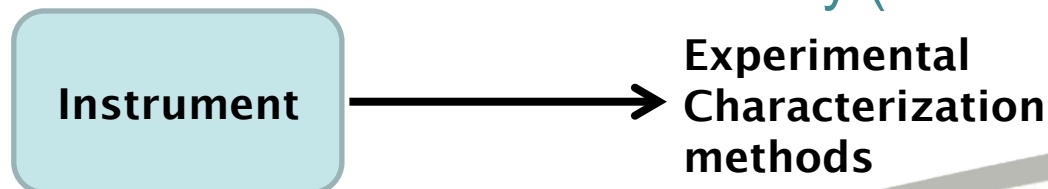
- Use the Vocab to annotate the CSMD entities
 - Particularly the Sample Entity



- Or better



- Also Instrument Entity (and/or Investigation)

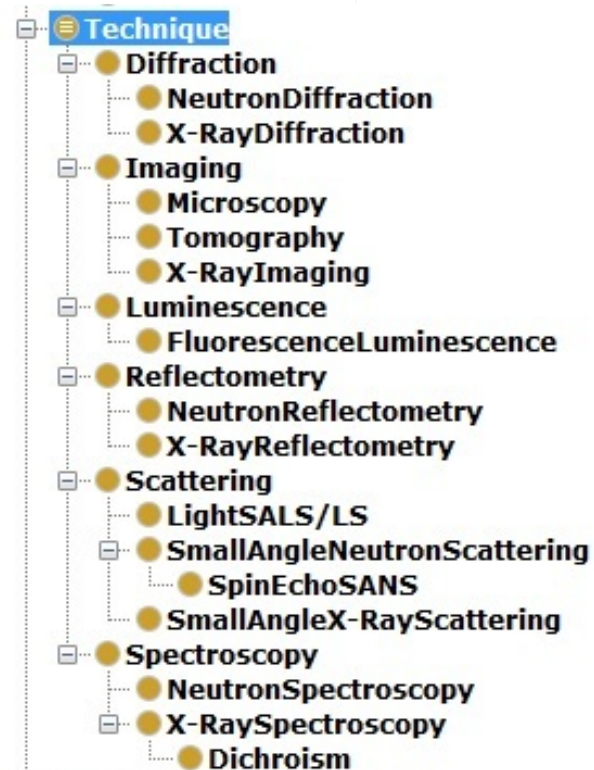
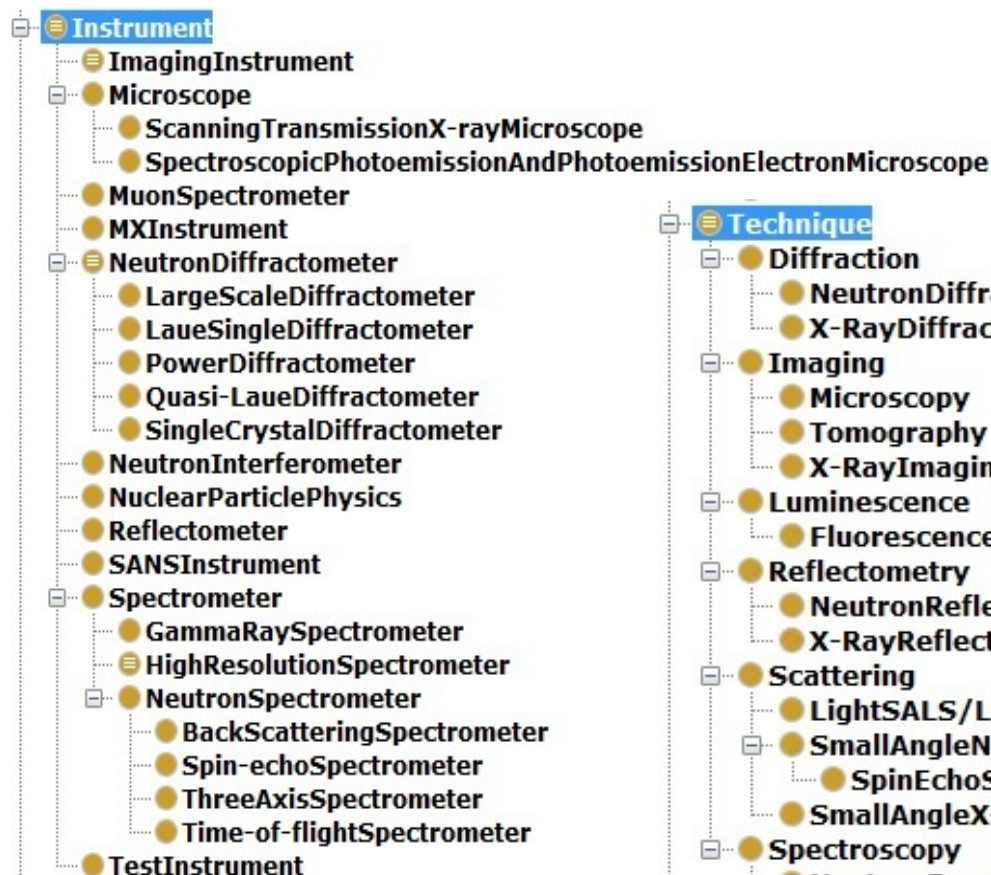
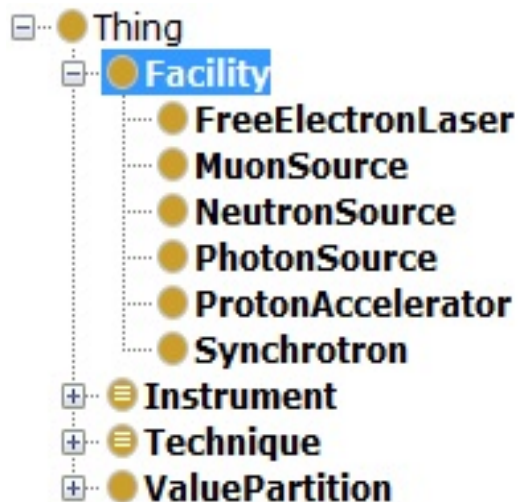


- Maybe Computational Methods and Software/Job
 - Though there is a conceptual difference



Facilities, Instruments, Techniques

- Classify facilities and instruments
- Provide a unique ID
- WG International Materials Resource Registry



Experimental Parameters

- This is an area not covered by the vocabulary
- Temperature, pressure, sample size/shape,
- Settings of instrument
 - Not appropriate for this vocab
 - Very important for the understanding of the experiment
- Use of NeXus - adds semantics to HDF5 files, *via*:
 - a metadata dictionary
 - a logical hierarchy of HDF5 groups
 - But still needs better consistency of parameter sets



Software Catalogue:

<https://software.pan-data.eu/>

The image shows two overlapping browser windows of the PaNdata Software Catalogue website. The left window displays the main homepage, while the right window shows a detailed view of the 'ABINIT' software entry.

PaNdata Software Catalogue (Main Page):

- Navigation: Browse Software, Institutes
- Search: search for software...
- PaNdata Software Catalogue description: PaNdata software catalogue is a database of software used mainly for data photon experiments. This database can be freely consulted. It gives an overview of software available for photon experiments and their use with respect to instruments at experiments. By registering and logging-in new software can be entered and it will appear after moderation.
- Buttons: Browse software, Add new software
- Recently added software section:
 - NeXpy**: NeXpy provides a high-level python interface to NeXus data and a simple GUI. It is designed to provide an intuitive interactive tool.
 - ANKAphase**: ANKAphase processes X-ray inline phase-contrast radiographs by reconstructing the projected thickness of the object(s) imaged. The tool uses a single-distance non-iterative phase-retrieval algorithm described in a paper by D. Paganin et al. J. Microsc. vol. 206 (2002). It has an easy-to-use graphical user interface and can be run either as a standalone application or as a plugin to ImageJ. It works on powerful clusters but also on your office laptop.
 - BONSU**: Bonsu is an interactive phase retrieval suite, designed for phase retrieval real-time visualisation in both two and three dimensions. It includes a graphical user interface and a command-line interface.

Software Detail View (ABINIT):

- Navigation: Browse Software, Institutes
- Search: search for software...
- Buttons: sign up, log in, Add new software
- Software List (Left):
 - INSTITUTES: All institutes
 - CATEGORIES: All categories
 - INPUT FORMATS: All data format inputs
 - OUTPUT FORMATS: All data format outputs
 - INSTRUMENTS / BEAMLINES: All instruments / beamlines
 - LANGUAGES: All languages
 - PLATFORMS: All platforms
 - LICENSES: All licenses
- ABINIT Software Description (Right):

ABINIT

ABINIT is a suite of programs for materials science, which implements density functional theory, using a plane wave basis set and pseudopotentials, to compute the electronic density and derived properties of materials ranging from molecules to surfaces to solids. It implements density functional theory by solving the Kohn–Sham equations describing the electrons in a material, expanded in a plane wave basis set and using a self-consistent conjugate gradient method to determine the energy minimum. Computational efficiency is achieved through the use of fast Fourier transforms, and pseudopotentials to describe core electrons. As an alternative to standard norm-conserving pseudopotentials, the projector augmented-wave method may be used. In addition to total energy, forces and stresses are also calculated so that geometry optimizations and ab initio molecular dynamics may be carried out. Materials that can be treated by ABINIT include insulators, metals, and magnetically ordered systems including Mott-Hubbard insulators.

Thank you and questions?

Brian Matthews

Brian.matthews@stfc.ac.uk



Science & Technology
Facilities Council