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

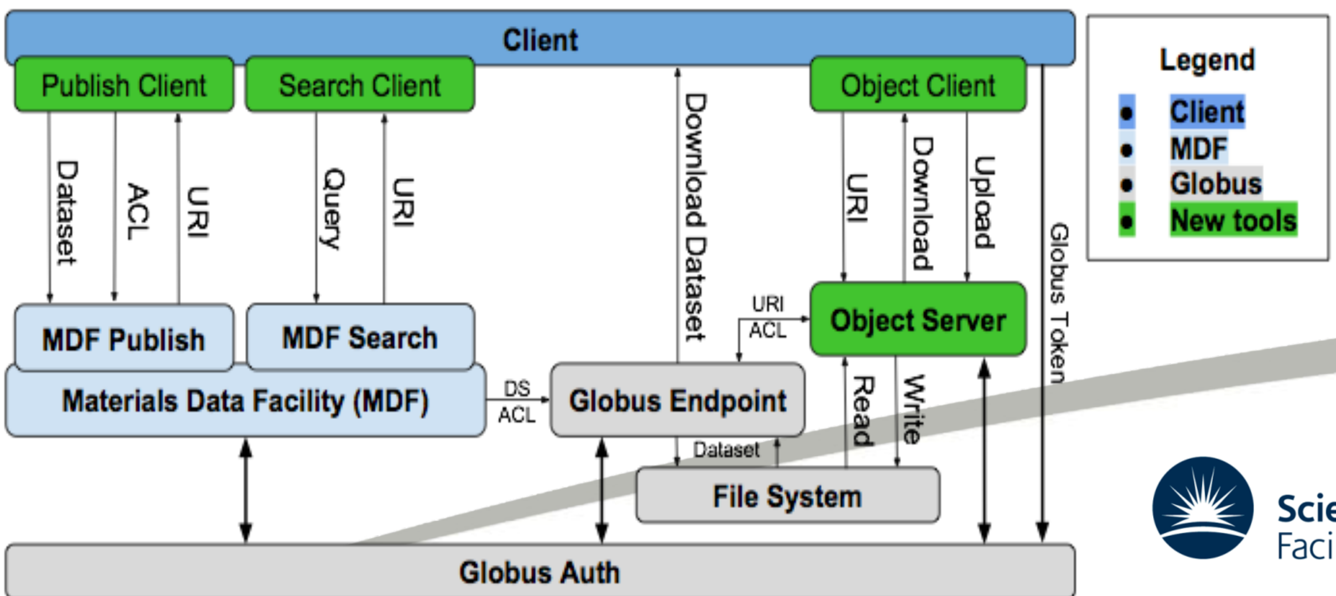
Materials science a major area

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



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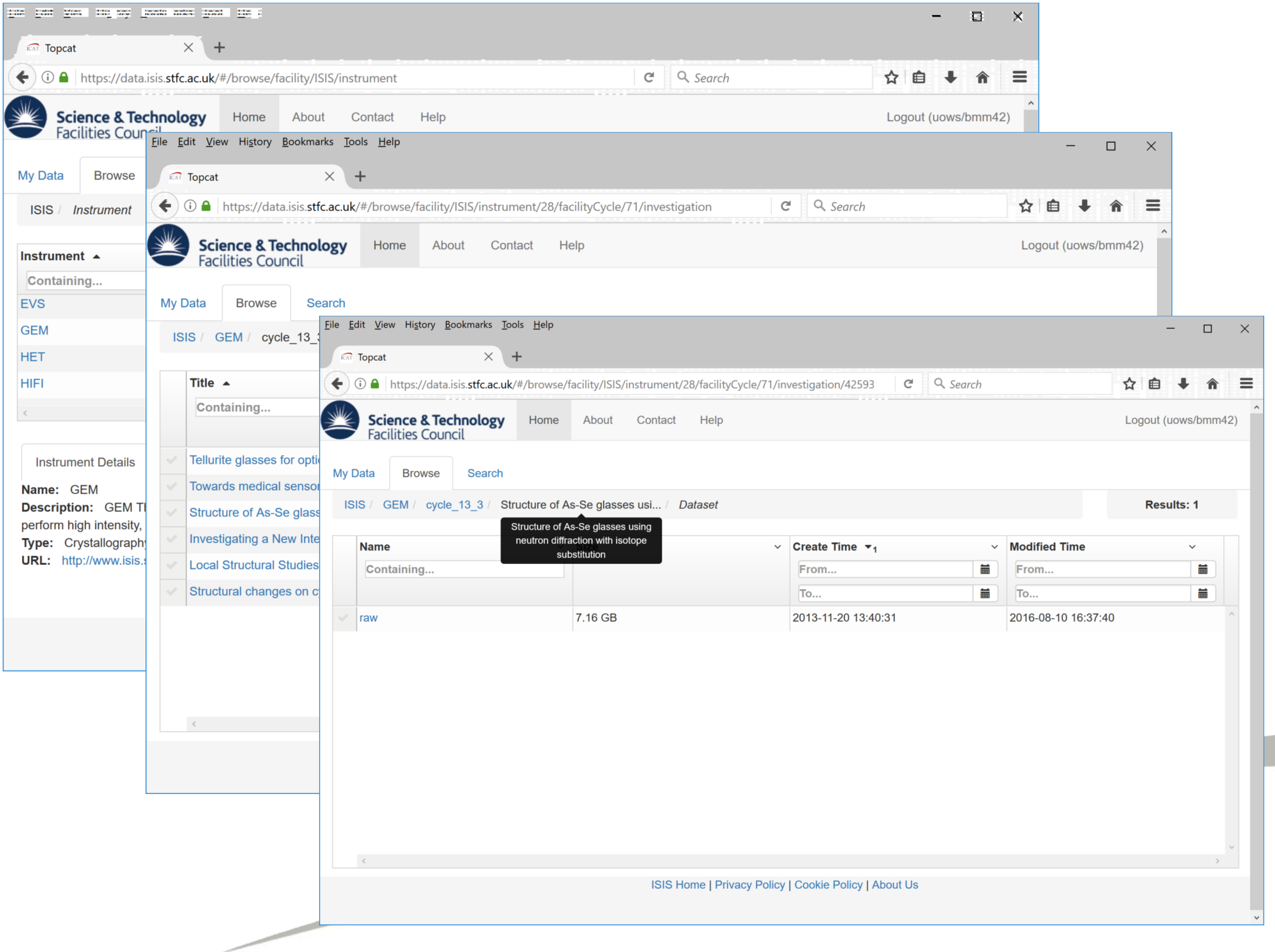
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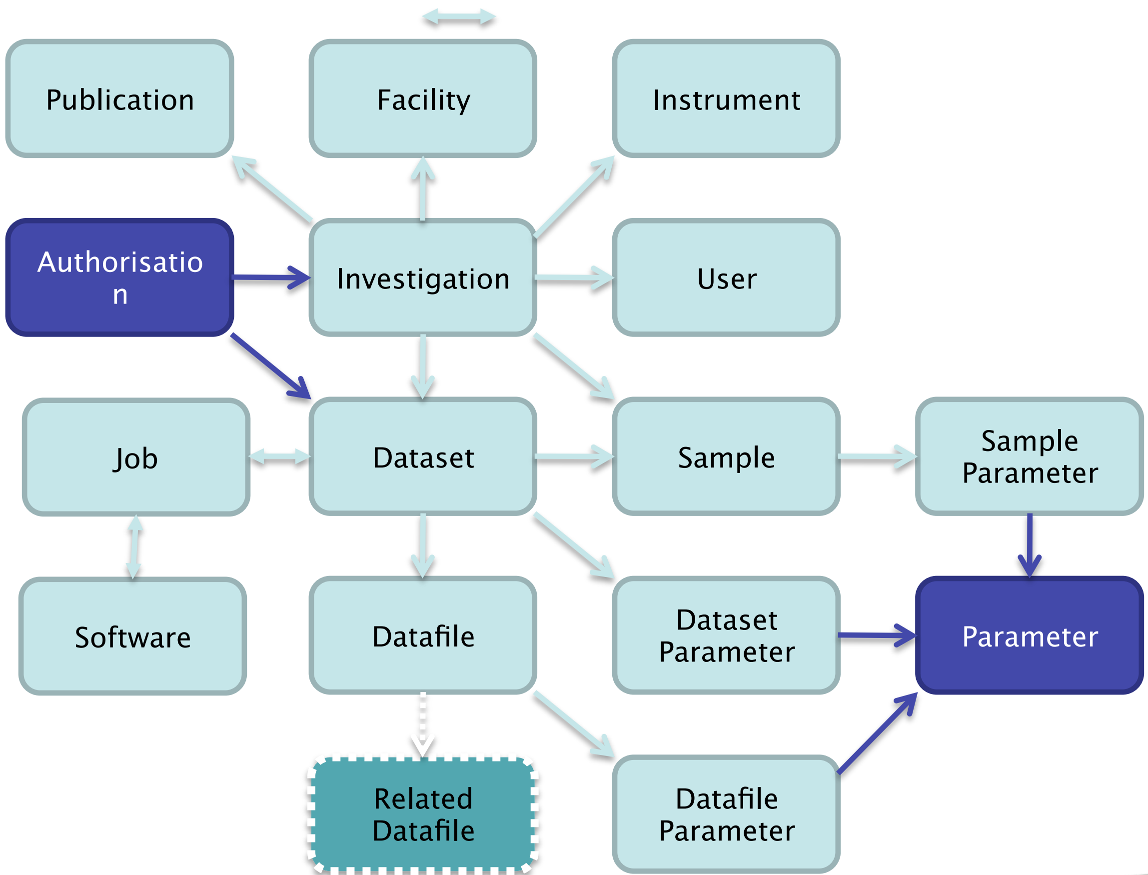
Core Scientific Metadata Model (CSMD)

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/

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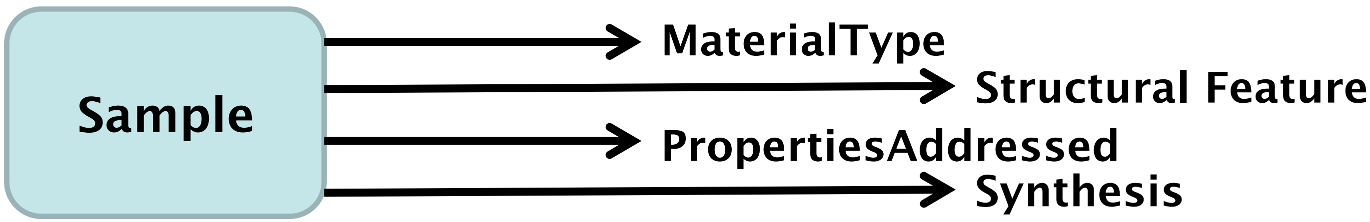
Materials vocab to describe resources

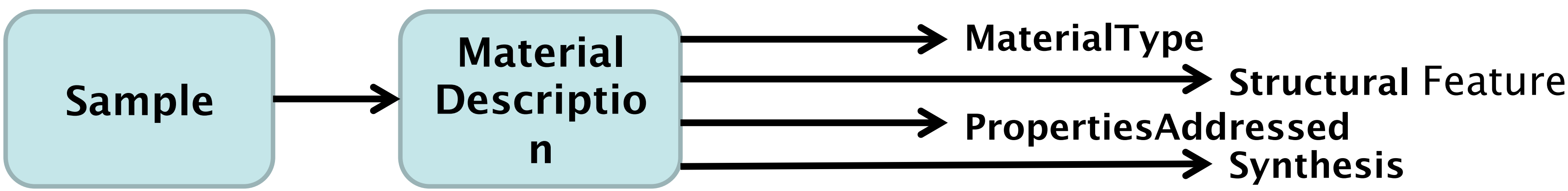
- Major categories
  - Material types
  - Structural features
  - Properties addressed
  - Experimental Characterization methods
  - Computational methods
  - Synthesis and processing
- But what do these categories describe ?

Adding Materials Vocab to CSMD Metadata Entities

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



  - Or better

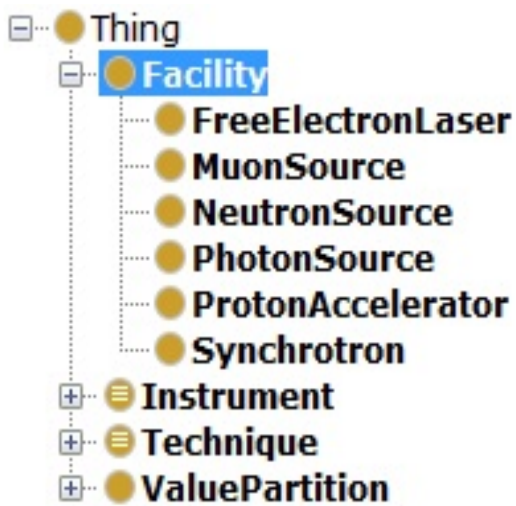


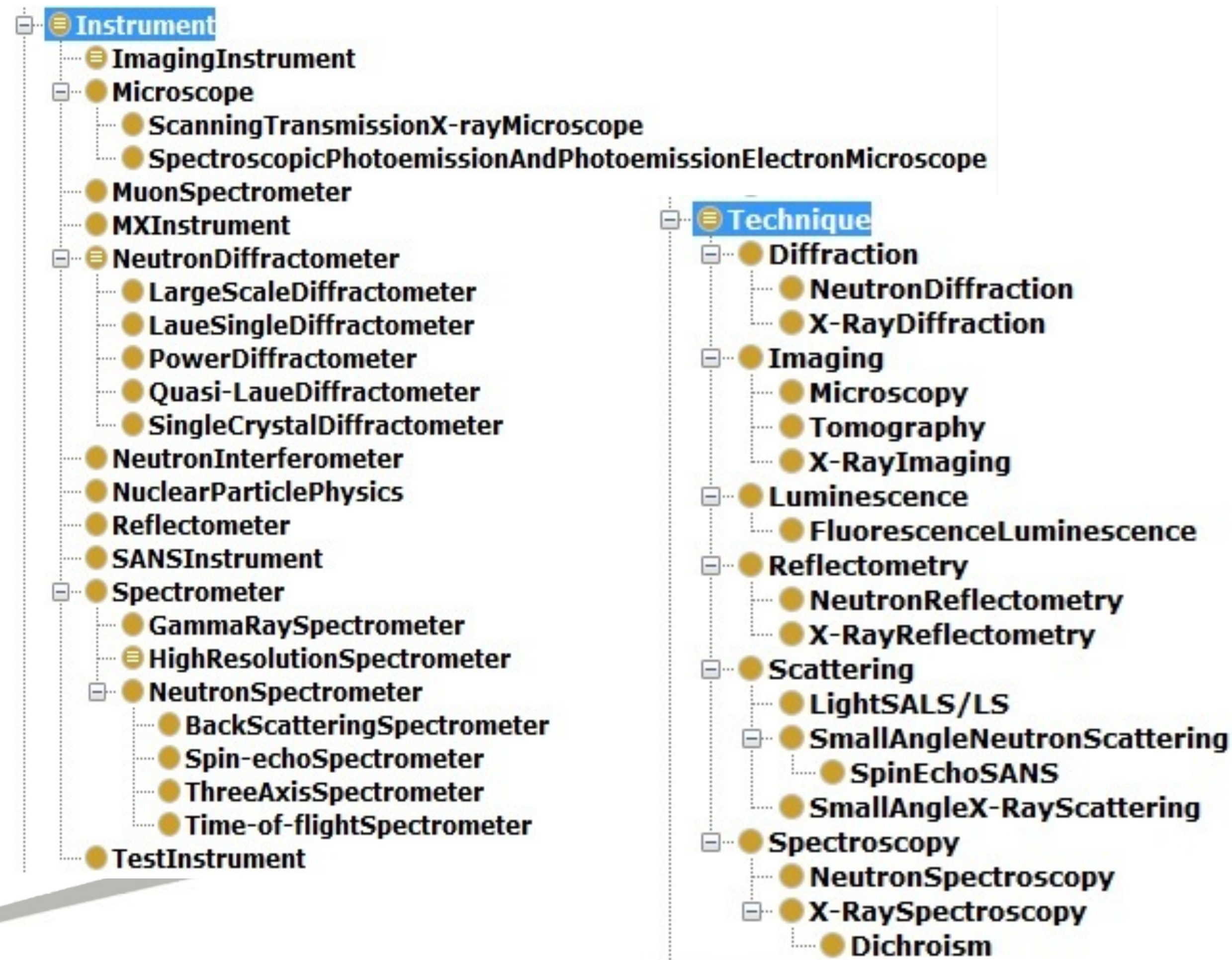
  - Also Instrument Entity (and/or Investigation)

  - 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 Registri**



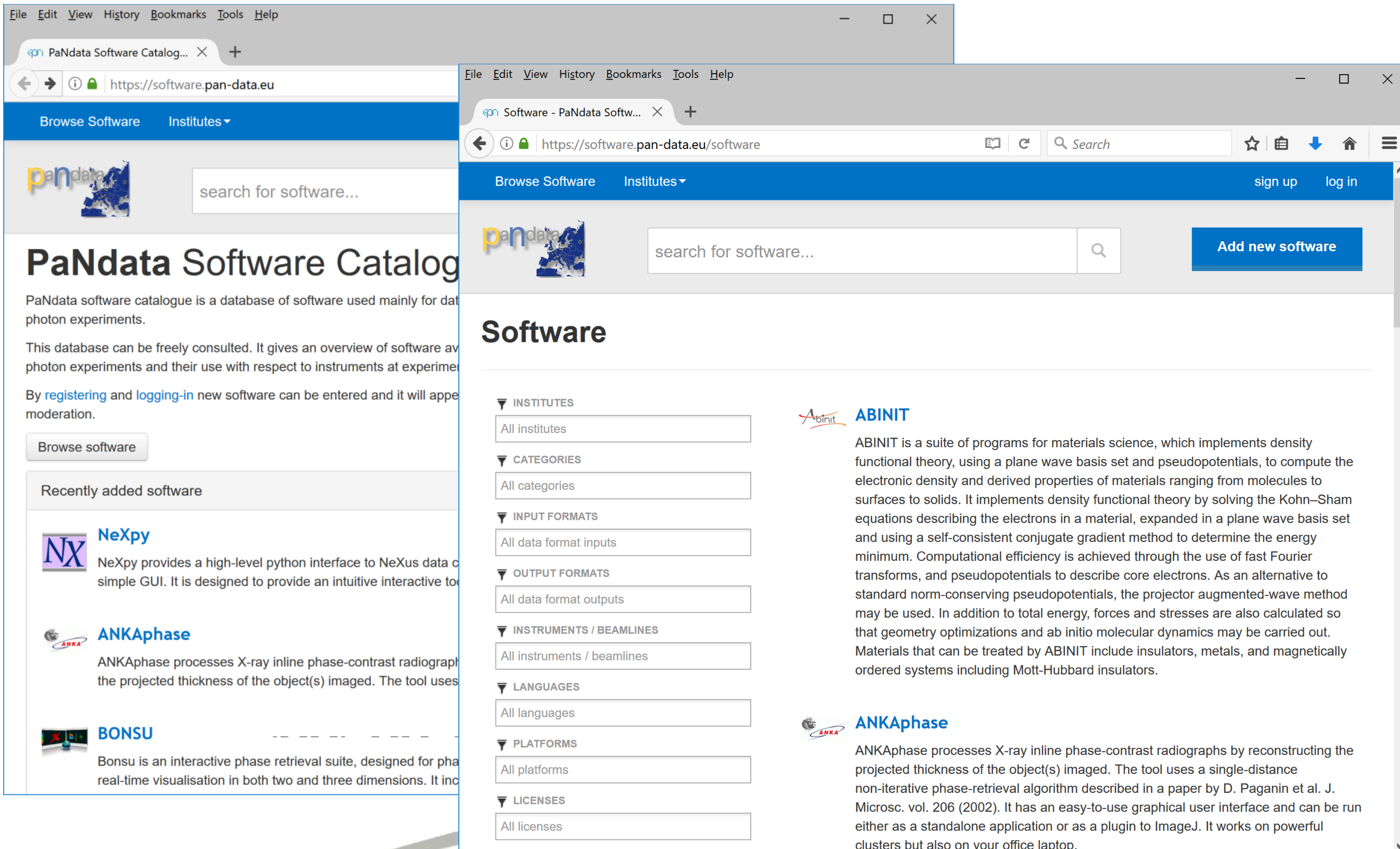


Experimental Parameters

- 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/



Thank you and questions?

Brian Matthews
Brian.matthews@stfc.ac.uk

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