

ICAT Workshop: Towards ICAT 4.3

Brian Matthews

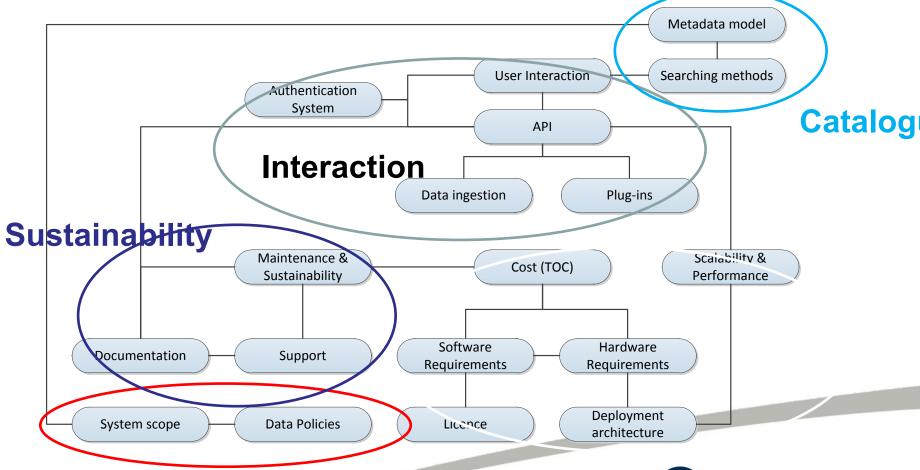
Scientific Computing Department



Evaluation Criteria



18 criteria for evaluating a data catalogue



Policies





ICAT Evaluation

| Authentication System | The authentication system is a plug-in. A suitable one can be done for Umbrella. Searching across multiple ICAT instances is possible. |
|----------------------------|--|
| Metadata model | The current one was designed with x-ray and neutron experiments in mind (captures the "Beamtime" concept). NXarchive [ref. to later text] has been designed specifically for ICAT. |
| Querying/Searching methods | Permits keyword based searching. Free-text is supported too. |
| Software Requirements | Enterprise Java technologies and Oracle RDBMS. The latest version can be deployed on MySQL too as requested by a PaNdata member facility. |
| User Interaction | The ICAT project has produced an interactive web-frontend to the system (Topcat). |
| Service API | The ICAT4 API is a layer on top of relational DBMS. The database is wrapped as a SOAP web service so that the tables are not exposed directly. When the web service interface definition (WSDL) is processed by Java then each data structure results in a class definition. |
| Hardware Requirements | According to the Software Requirements. |
| | Facilities Council |



ICAT Evaluation



| Documentation | ICAT is well documented. There is no up-to-date user guide for Topcat but there is a website and wiki for the project (http://code.google.com/p/icatproject/). |
|----------------------------------|--|
| Support | The ICAT team is providing the PaNdata consortium with extensive support. Members participate in regular teleconferences and meetings where current and future developments are discussed. There is formal agreement between the ICAT project and PaNdata ODI WP4. |
| Licence | Open source - FreeBSD. |
| Data Policies | N/A. |
| Total Cost of Ownership (TCO) | The system is open source and its current version requires only open-source or free technologies. It offers good and responsive support. It will be used among the PaNdata partners as a common system. |
| Scalability and Performance | An existing installation of Petabyte scale reports satisfactory performance. |
| Data Ingestion | The API permits simple data ingestion. |
| Additional Services and Plug-ins | It is open source, has an API that is SOAP based, and is modular. |
| Deployment Architecture | Mostly single server instances but a federated distribution of ICATs is possible. This would enable the web portal (Topcat) to be on top of the API. |
| Maintenance and Sustainability | ICAT follows good software sustainability practices and has been reviewed by the Software Sustainability Institute. |
| Specialisation and Systems Scope | The system is specialised as it mostly realises a data catalogue service. Its scope is well suited for scientific data. |

Further PanData Requirements CAT



| Authentication System | Should enable DCS operations across PaNdata facilities. Should be easily integrated with the existing local authorisation and file systems. |
|----------------------------------|---|
| Metadata model | Should be extendible and support discipline specific annotations. Unique identifiers to allow for citation (DOIs). |
| Querying/Searching methods | Should permit keyword based searching. |
| Software Requirements | The DCS should be based on a widely-used DB. |
| User Interaction | Should provide the end-user with a web-portal. |
| Service API | An API that permits at least all the operations that can be done through the portal. |
| Hardware Requirements | N/A |
| Documentation | Documentation and user-guide for the API and the web-portal. |
| Support | N/A |
| Licence | N/A |
| Data Policies | N/A |
| Total Cost of Ownership (TCO) | N/A |
| Scalability and Performance | Fast enough to permit interactive work (web-portal) |
| Data ingestion | N/A |
| Additional Services and Plug-ins | Upload/download/delete of files, change permissions (through the web portal). Support for a Workflow system. |
| Deployment architecture | N/A |
| Maintenance & Sustainability | N/A |
| Specialisation and Systems scope | Virtual labs as described in D5.1 and scientific applications related to the participating institutes. |

Further PanData Requirements [AT



| Authentication System | Easy integration with the Umbrella system as described in D3.1. |
|----------------------------------|---|
| Metadata model | A model that covers the metadata present in an advanced scientific data file format (NeXus). |
| Querying/Searching methods | Querying value ranges. Use of Tags. |
| Software Requirements | Server-class Linux OS and reliance on open source solutions. |
| User Interaction | As in D5.1. |
| Service API | API bindings for languages as C++, Java, and Python. Ideally, bindings for high level numerical computing environments (Matlab/IDL) so that the users can query the system and index post-processed data too. |
| Hardware Requirements | Server-class systems. |
| Documentation | As in D5.1. |
| Support | Support for both usage and development from the system's development team. |
| Licence | Open source. |
| Data Policies | It should not conflict with the PaNdata Europe Data Policy. Ideally should permit automated policy enforcement actions like changing the access of certain data to Public after a predefined time. |
| Total Cost of Ownership (TCO) | Follow the Compliance to Standards (i.e. using a common system among similar institutes). Pay no fees for support and proprietary software. No high maintenance costs after the end of the project. |
| Scalability and Performance | Should scale well when additional hardware is added and cope with the data flow of each member facility. |
| Data ingestion | Sample code for data ingestion through the API. |
| Additional Services and Plug-ins | Possible interaction with workflow systems (e.g. Taverna, Kepler) and data provenance frameworks. |
| Deployment architecture | Should permit multiple instances (distributed across the institutions) able to return cross-facility search results. |
| Sustainability | The system development team should have high maintenance and software sustainability standards. |
| Specialisation and Systems scope | Software specialised on scientific data without additional technologies like Grid frameworks and complicated certificate based systems. |



PaN-Data WP4: Next Steps

- Task 4.2: Serially, deploy the chosen metadata catalogue solution in the legacy context of the collaborating facilities
 - ICAT being rolled out across a number of the facilities
 - ISIS, DLS, CLF, ILL, ELETTRA, ESRF, ...
 - Regular Service Verifications
- Requirements and implementation influenced by the facilities
 - Open source collaboration: ICAT/PaNData
 - http://www.icatproject.org/
 - http://code.google.com/p/icatproject/





SSI Review

- Governance
- Communications
- Process
- Policies
- Support
- Infrastructure



What might go in ICAT 4.3 – and beyond



- Remove the ICATCompat interface
- Improved error messages for less common errors
- Add a Run entity
- Improve notification to include which operation was being used and to make it a better match users needs while imposing minimal overhead
- Allow a rule to specify that an authz plugin should be applied
- Introduce a namespace to relate to types instead of facility. The namespace should have many to many relationship to a facility



Down the line?



- Controlled vocabulary;
 - For searching/reporting
 - keywords, facilities, instruments, techniques
 - · parameters and parameter sets
 - samples
- Standard
 - Dataset types
 - Investigation types
 - Datafile formats (mime-types)
 - Groups and their rules (Admin, data ingestors, Instrument scientists ...)
- Integration with frameworks
 - Mantid, Dawn
 - Workflow Engine
 - Access to PanSoft software catalogue
- Programming language bindings
 - Java, Python, ??
- Extend the component architecture
 - Light-weight laboratory use
 - Simple web interface
 - ICE
 - Command Line

- XML Ingest
 - Example data: script to set up with virtual data, Virtual machine
- Screencast of full installation
- Linked Data
- Notification and reporting examples
- Handling more than one facility within one ICAT.
- Common data server interface (IDS2)
 - Managing large files
 - Handing off to a suitable protocol.







Feedback

- What would you like to see?
- What can you contribute?

JOIN IN!

http://www.icatproject.org/ http://code.google.com/p/icatproject/ icatgroup@googlegroups.com icat-developers@googlegroups.com

