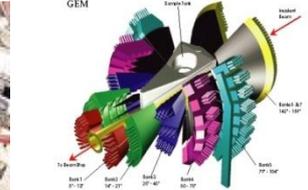


# Collaborative Information Management in Scientific Research Processes

**Shirley Crompton**, Brian Matthews, Erica Yang : STFC Scientific Computing  
Cameron Neylon : STFC ISIS  
Simon Coles : University of Southampton, School of Chemistry

# Science and Technology Facilities Council

- Research Funder
  - Provides large-scale scientific facilities for UK Science
    - ISIS, Diamond, CLF...
- Scientific Computing
  - Facilities e-Infrastructure
    - ICAT Data Catalogues
    - E-Publications Archive
    - Petabyte Data Store
  - Active contributor to data management, digital data preservation research and infrastructure building
    - ICAT, SRF, Scidip-ES, SCAPE ...
    - PanDATA, APARSEN...

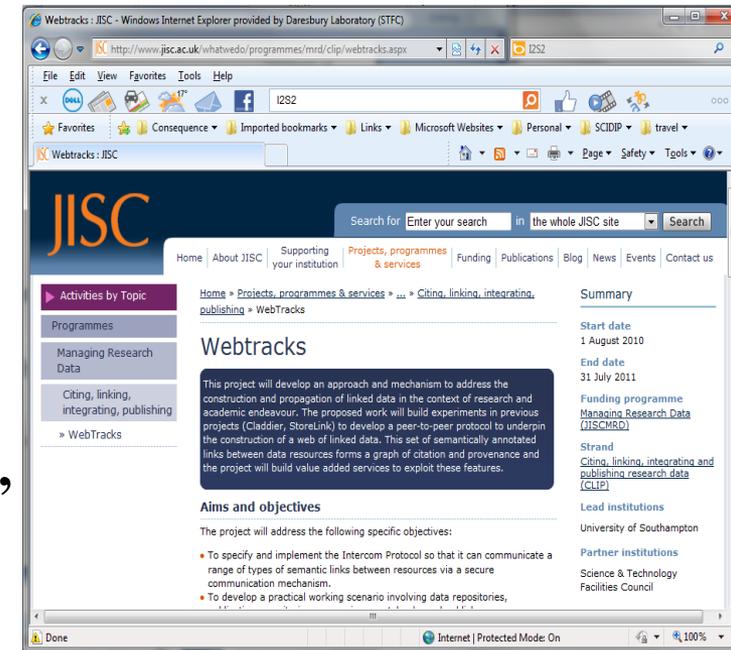


# Overview

- The Webtracks project
- Our motivations
- The Webtracks approach
- Webtracks exemplars
- Future Work : SRF
- Summary

# Webtracks Project

- Web-scale link TRACKing for research data and publicationS
- Develop an approach and mechanism for constructing and propagating linked data in the context of research activities
- Building on prior work in Claddier, StoreLink on citation linking
- Collaboration between:
  - Chemistry Dept, Southampton University
  - STFC Scientific Computing
- Funded by the JISC Managing Research Data (MRD) Programme



<http://www.jisc.ac.uk/whatwedo/programmes/mrd/clip/webtracks.aspx>

# The Scientific Research Process (1/2)

Diverse tools/services + Objects

Experiment

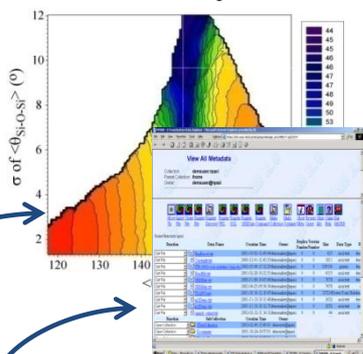


Raw data

ICAT  
Data Catalogue



Data analysis



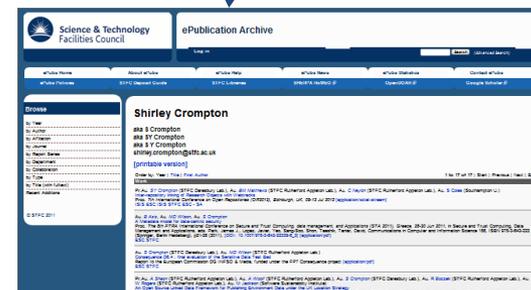
Protein model



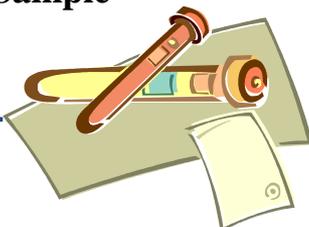
Publication



Publication



Sample



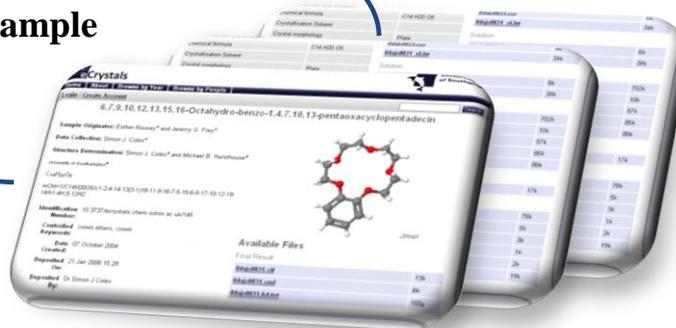
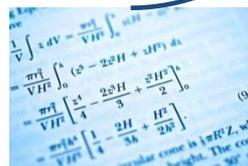
Describe sample

Describe algorithm

Describe derived data



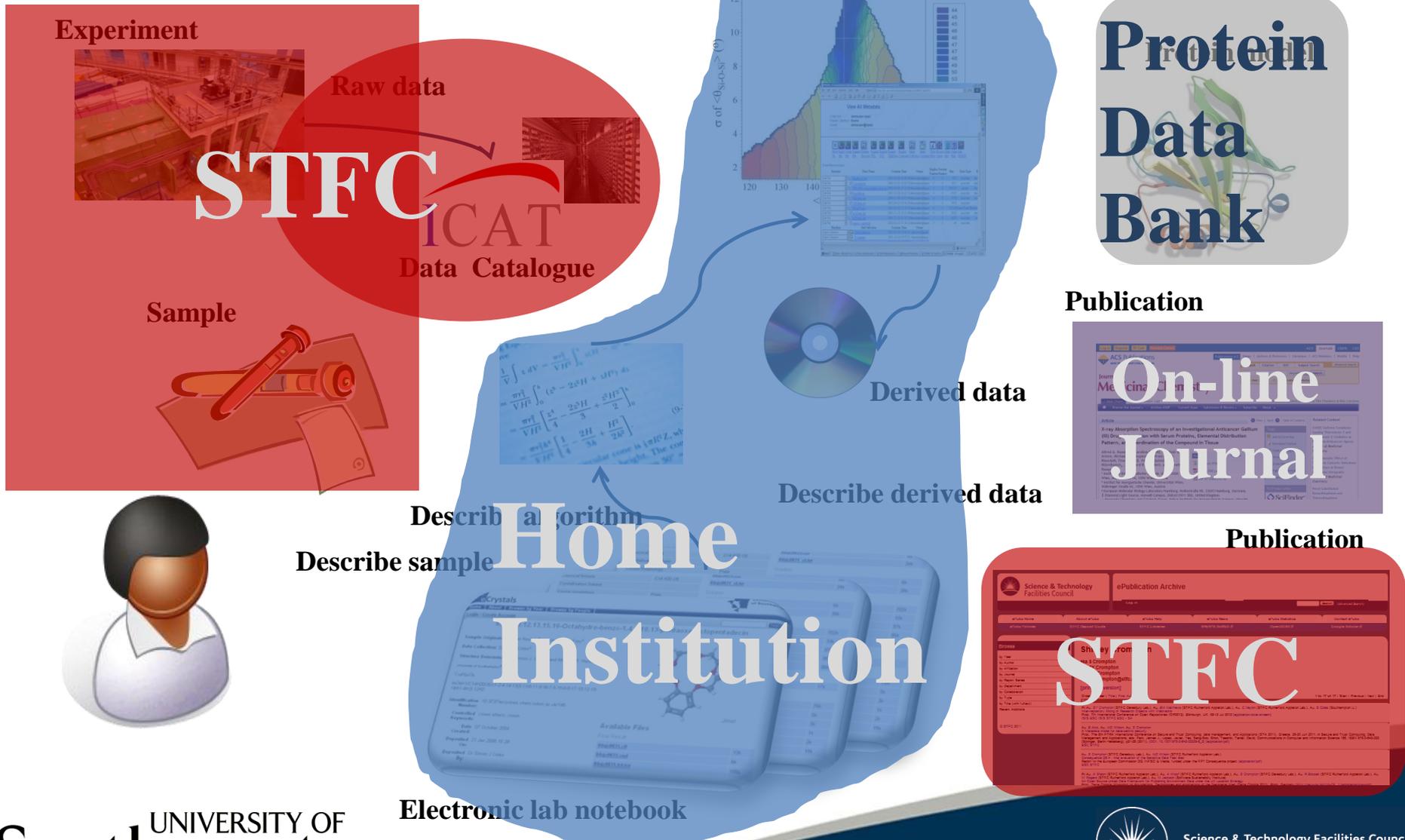
Derived data



Electronic lab notebook

# The Scientific Research Process (2/2)

## Contents Dispersed



# Adding Structured Citation Links

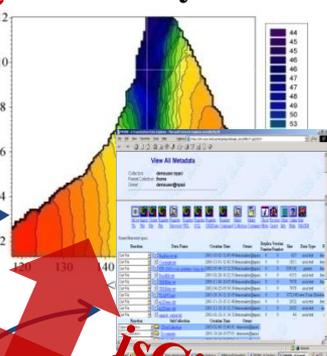
Experiment



Raw data

provides Data For

Data analysis



documents is Documented By

Publication

has Sample

ICAT Data Catalogue

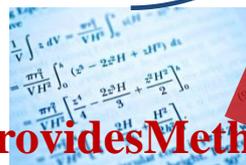


is Cited As Data Source

Derived data



provides Method For



Describe derived data

Describe algorithm

Describe sample

cites is Cited By

Publication

has PI

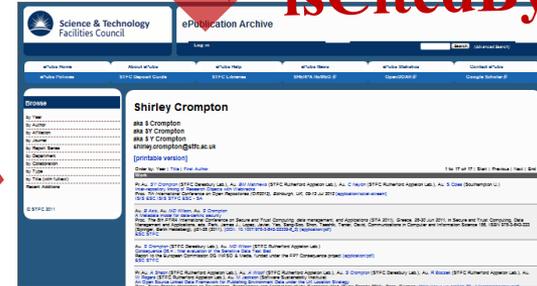
Sample



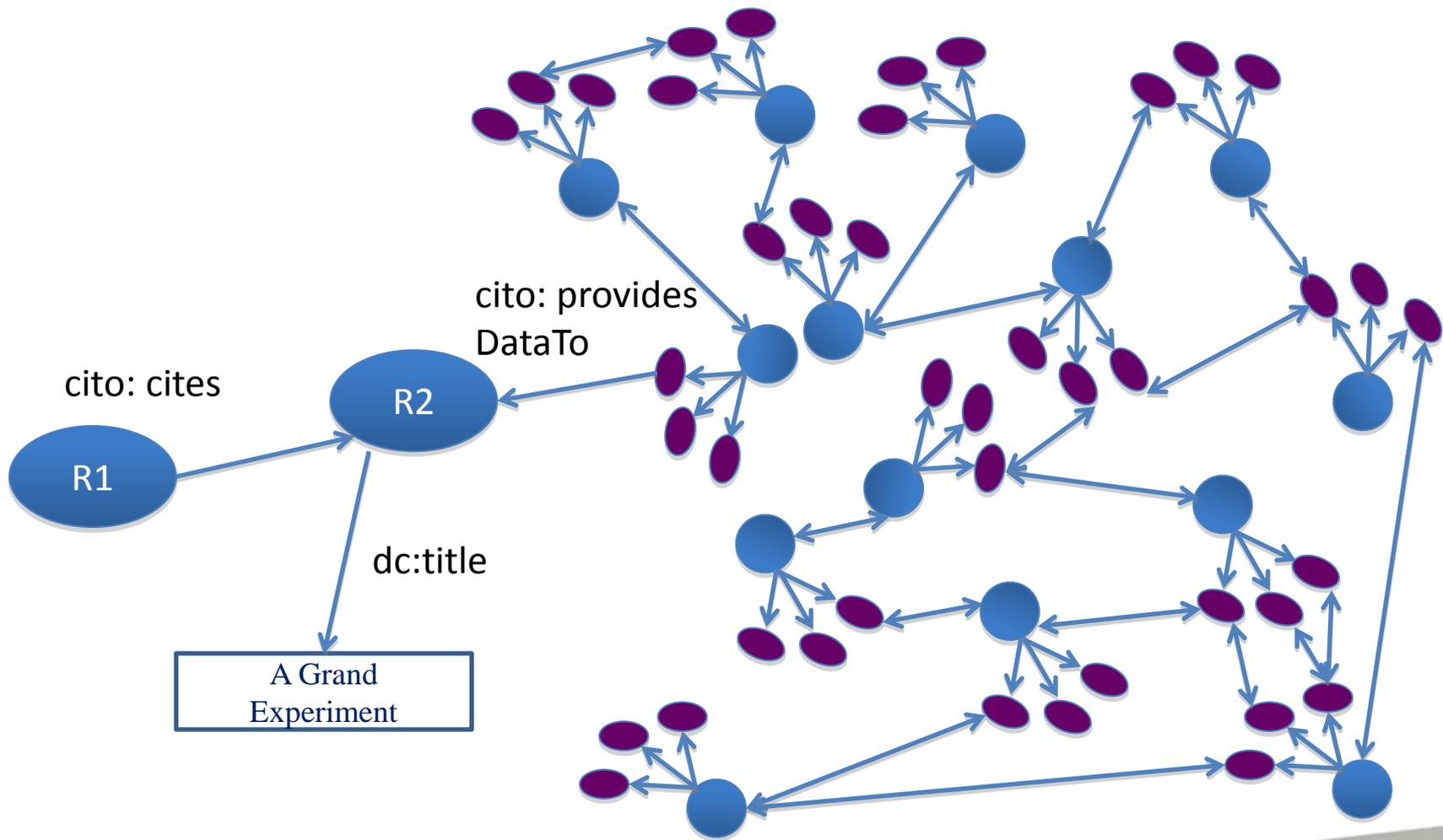
creator



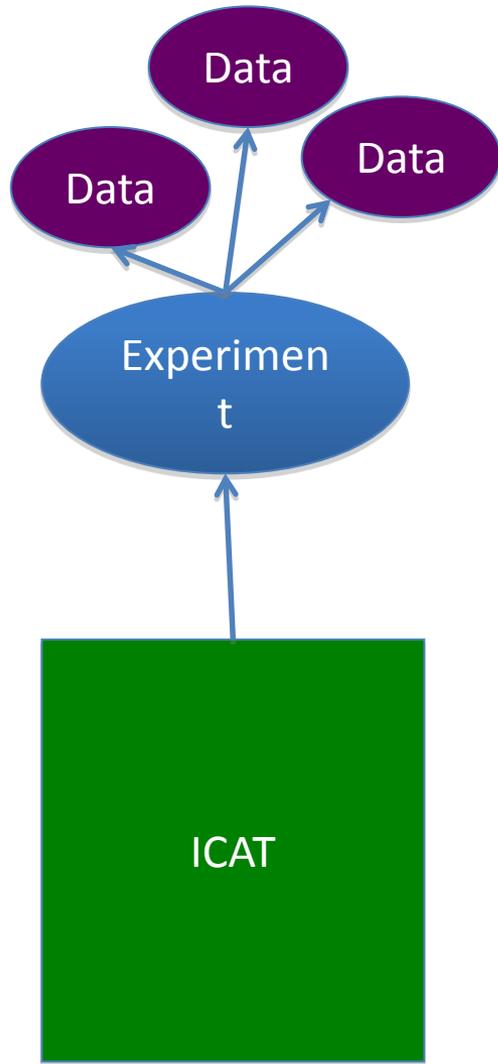
Electronic lab notebook



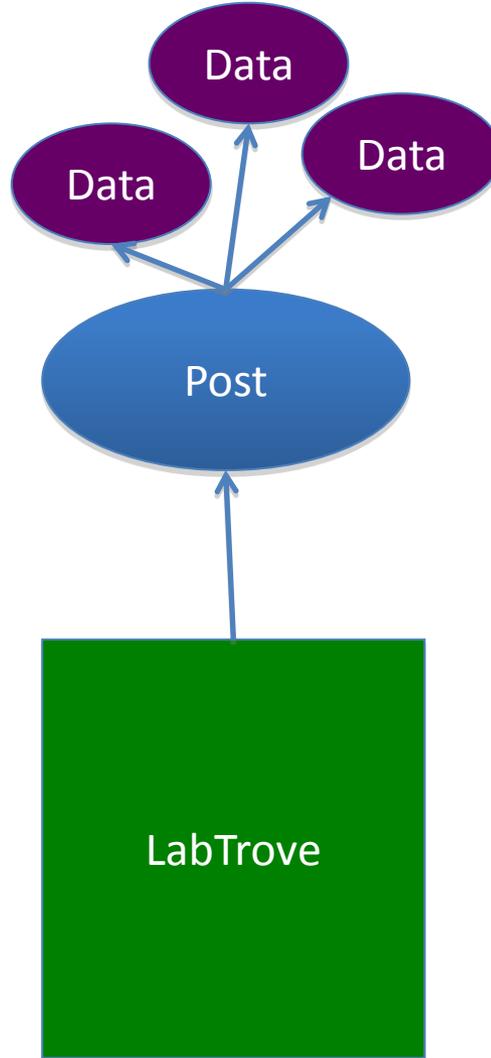
# A Federated Web of Research Objects



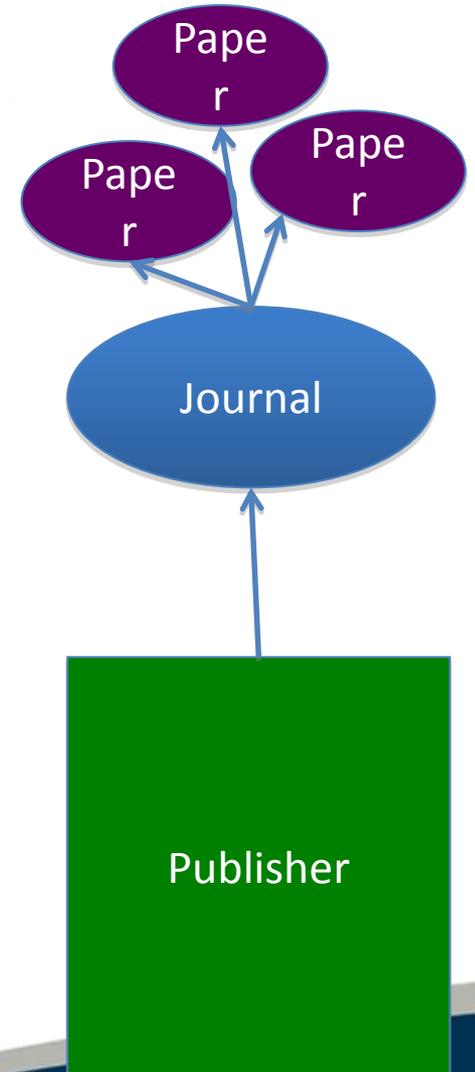
If we allow repositories to communicate ....



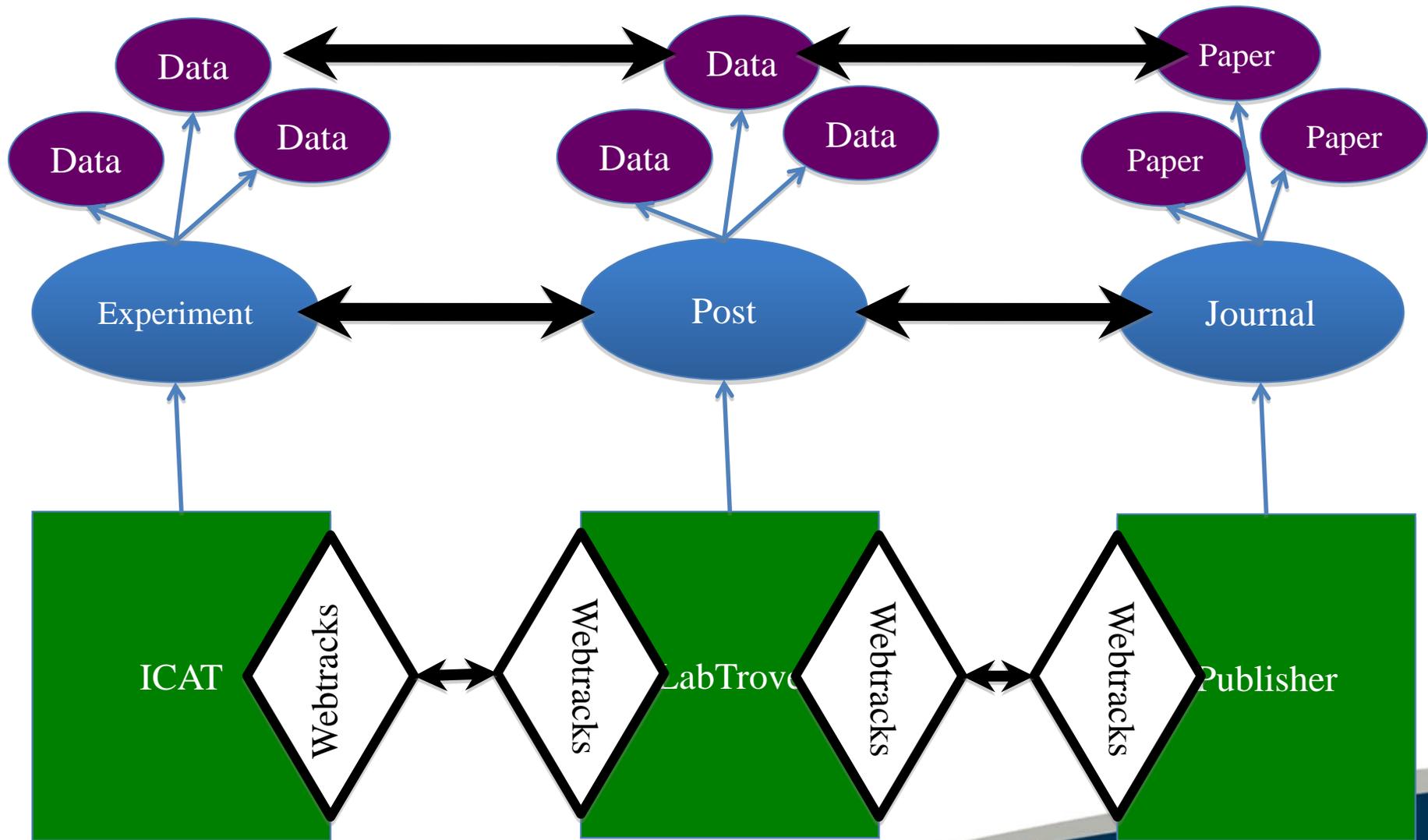
?



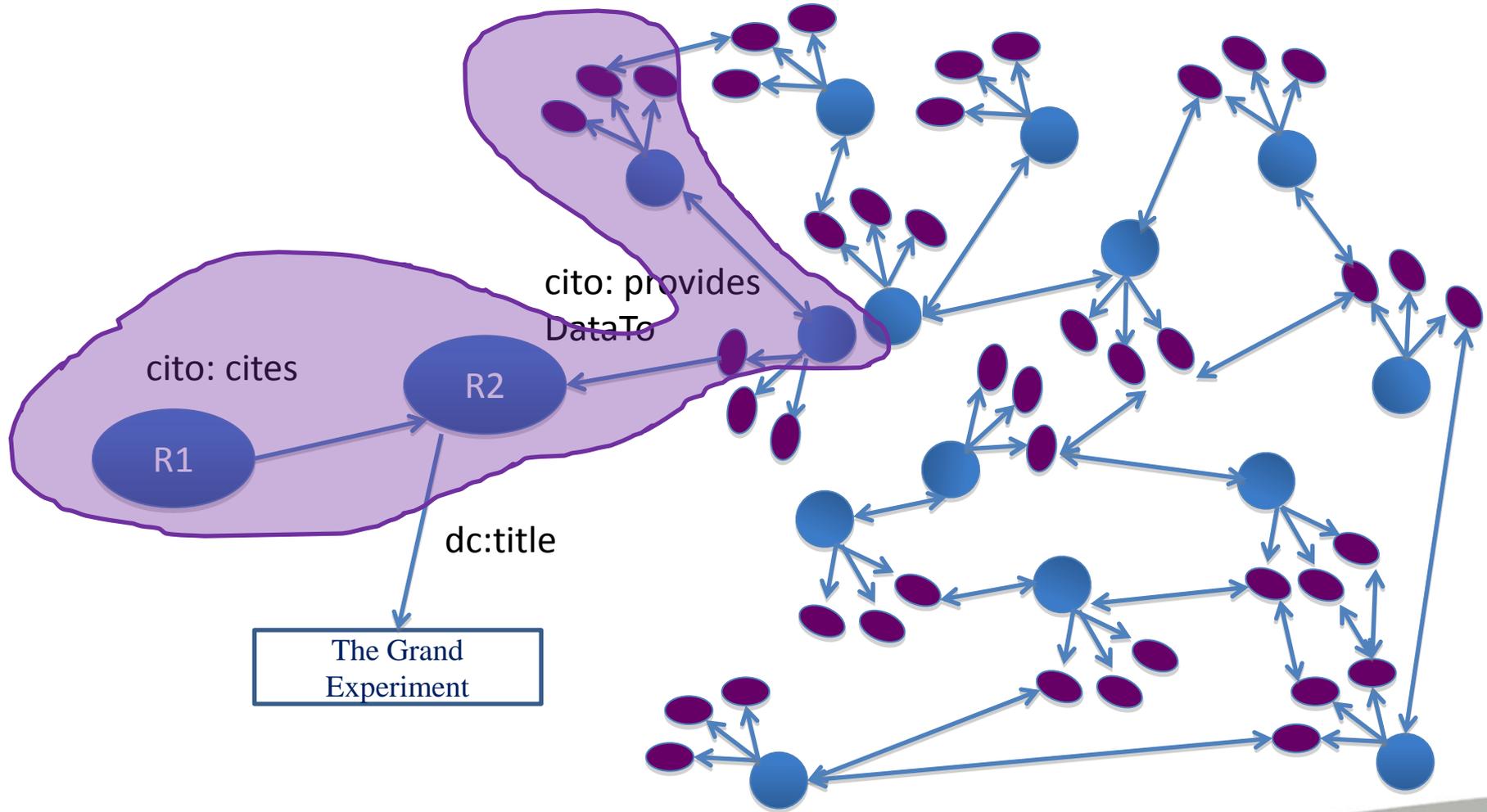
?



# If we allow repositories to communicate ....



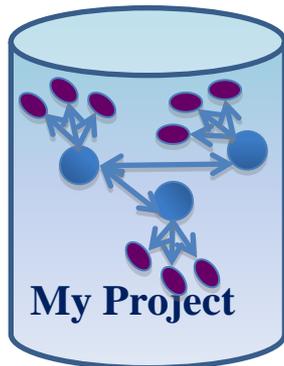
# Querying the RDF graph to form Research containers



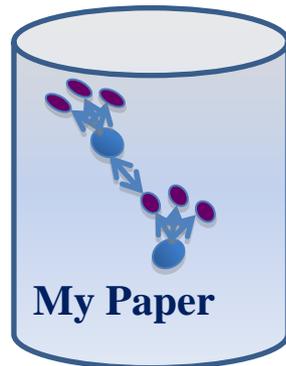
# Research containers

Fragments of Annotated RDF graph capturing specific relationship between on-line research objects

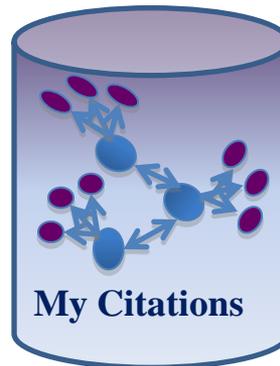
Example usages....



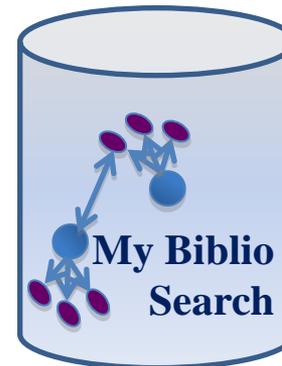
**Provenance tracing**



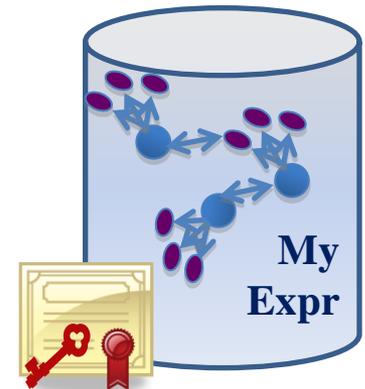
**Discovery of related objects**



**Impact factor**



**Research resource**



**Trusted publication**

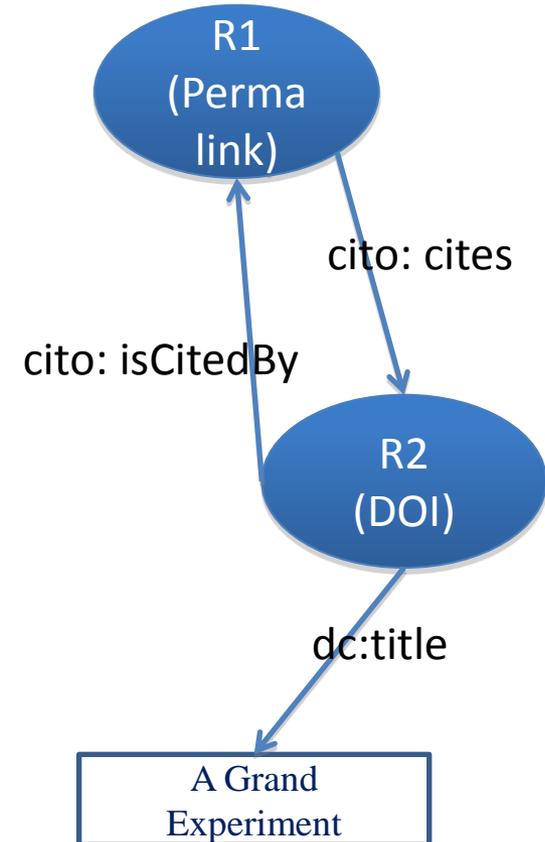
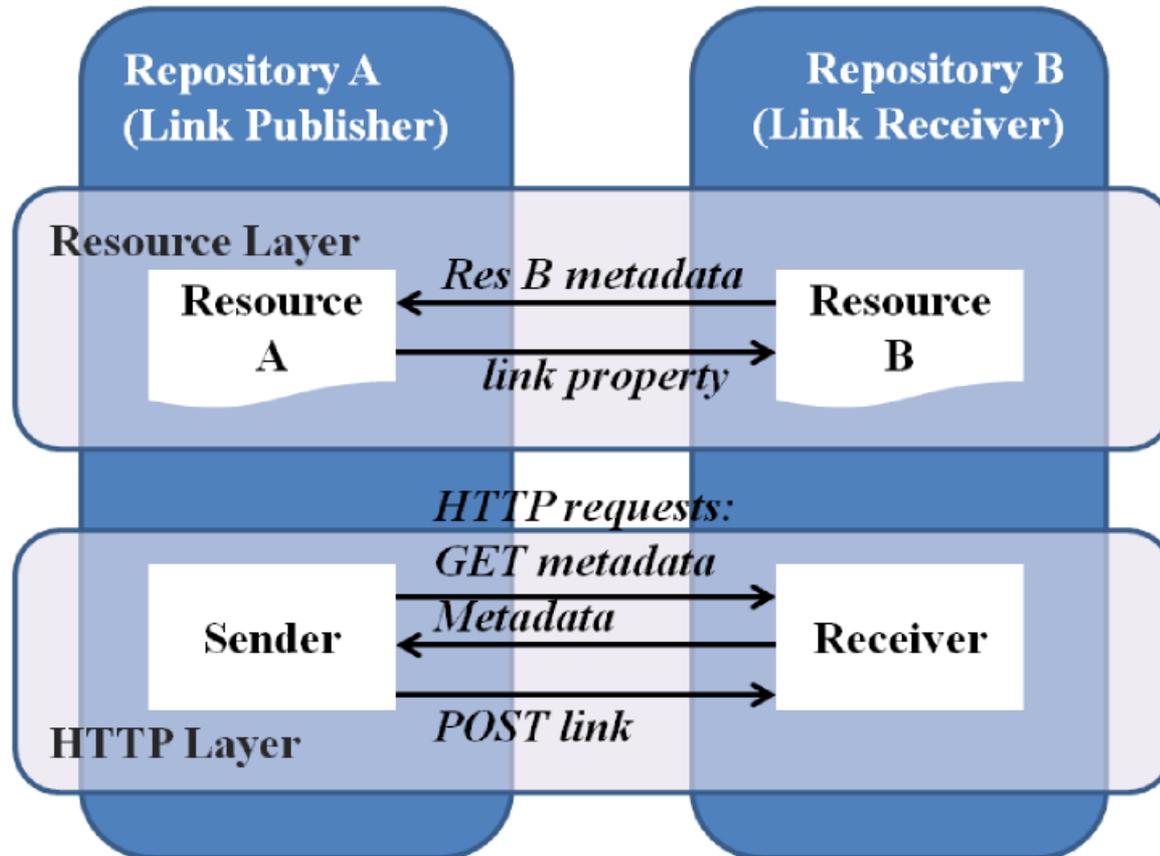
# The Webtracks Approach

- Inter-repository communication protocol
  - Based on Storelink
- Webtracks Java Restlet application

# Related protocols

- Trackbacks
  - track distributed blog ‘conversations’
  - With fixed semantics
- Semantic Pingback
  - RPC protocol
- Salmons
  - RSS protocol, non-RDF approach
- Claddier/Storelinks
  - P2P, no centralised service
  - Support fixed formats of metadata and link semantics
- ....

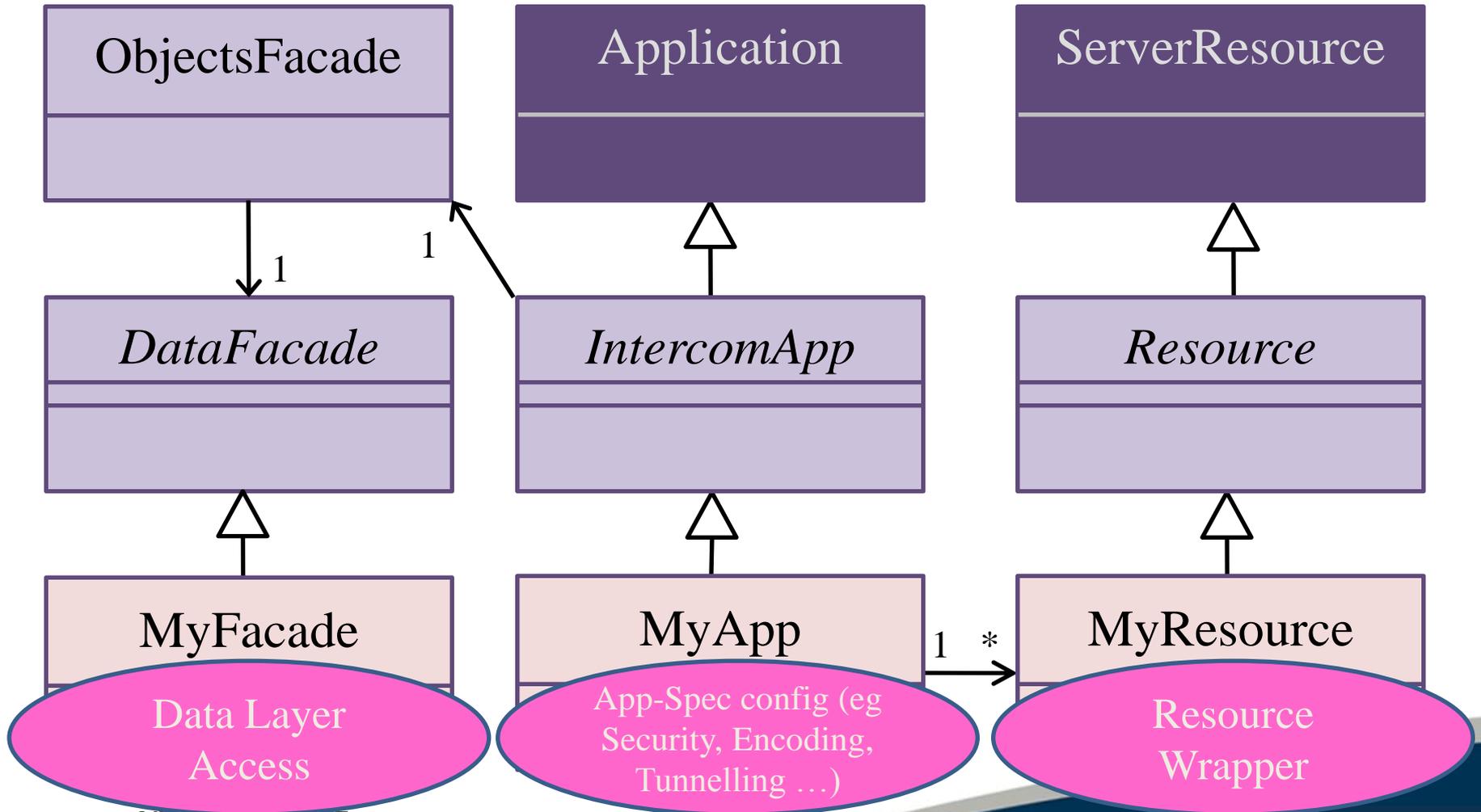
# The Webtracks InteRCom protocol



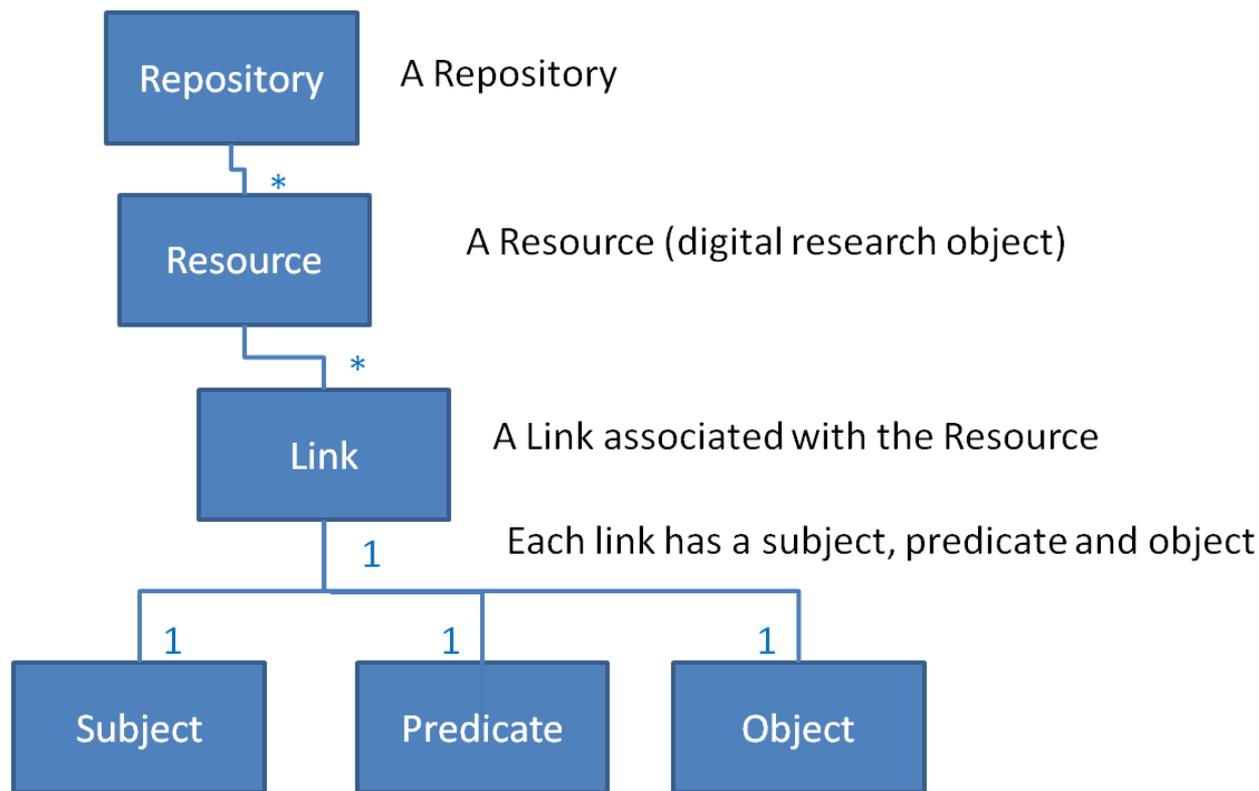
# Architecture (main classes)

(based on Restlet Framework)

Extension point



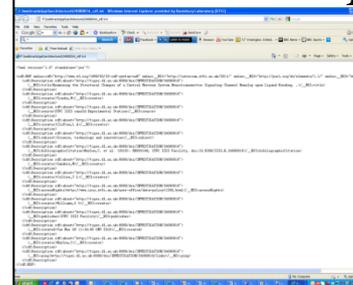
# Webtracks Resource Info Model



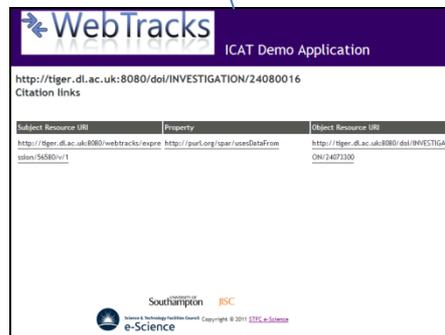
# Webtracks-Icat Exemplar



Investigation Resource  
 - DOI Landing Page  
 - HTML rep with RDFa



RDF rep



Links Resource  
 - HTML rep with RDFa

# Webtracks-Epubs Exemplar

## Epubs

WebTracks Epubs Demo Application

Some remarks on the analysis of the decay density matrix of mixed scalar-vector-tensor boson systems

HTTP URI - <http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v1>

Publication Title	Nucl Phys B
Contributor	R. L. Sekulin
Year	1973
Volume	56
Start Page	227
ISSN	05503213
BibCitation	R. L. Sekulin, Some remarks on the analysis of the decay density matrix of mixed scalar-vector-tensor boson systems, Nucl Phys B 56, 227 (1973)
Webtracks Ping	<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v1/links">http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v1/links</a>

Southampton e-Science JSC

## Expression Resource -HTML rep with RDFa

```

<!-- RDFa -->
<!-- Description -->
<!-- Title -->
<!-- Author -->
<!-- Year -->
<!-- Volume -->
<!-- Start Page -->
<!-- ISSN -->
<!-- BibCitation -->
<!-- Webtracks Ping -->

```

## RDF rep

WebTracks Epubs Demo Application

<http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v1>

Citation links

Subject Resource URI	Property	Object Resource URI
<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v1">http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v1</a>	<a href="http://purl.org/par/usesDataFrom">http://purl.org/par/usesDataFrom</a>	<a href="http://tiger.dl.ac.uk:8080/dot/INVECTIGA/TXON/24380016">http://tiger.dl.ac.uk:8080/dot/INVECTIGA/TXON/24380016</a>
<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v1">http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v1</a>	<a href="http://purl.org/par/cites">http://purl.org/par/cites</a>	<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/21612/v1">http://tiger.dl.ac.uk:8080/webtracks/expression/21612/v1</a>
<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/21612/v1">http://tiger.dl.ac.uk:8080/webtracks/expression/21612/v1</a>	<a href="http://purl.org/par/cites/isCitedBy">http://purl.org/par/cites/isCitedBy</a>	<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v1">http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v1</a>

Southampton e-Science JSC

## Links Resource - HTML rep with RDFa

# InterCom Citation Linking



ICAT DOI Landing Page

RE800186

Investigation title: Examining the Structural Changes of a Central Nervous System Neurotransmitter Signaling Channel Homolog upon Ligand Binding.

Creators: Neylon,C; Clifton,L A; Collier,J L; Tracks,W; Sanders,M; Williams,G O

Object type: INVESTIGATION

DOI: 10.5280/ISIS.E.24080016

HTTP URI: <http://tiger.dl.ac.uk:8080/doi/INVESTIGATION/24080016>

Webtracks Ping: <http://tiger.dl.ac.uk:8080/doi/INVESTIGATION/24080016/ping>

Icat Investigation Links Page

http://tiger.dl.ac.uk:8080/doi/INVESTIGATION/24080016

Citation links

Subject Resource URI	Property	Object Resource URI
<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1">http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1</a>	<a href="http://purl.org/spar/usesDataFrom">http://purl.org/spar/usesDataFrom</a>	<a href="http://tiger.dl.ac.uk:8080/doi/INVESTIGATION/24073300">http://tiger.dl.ac.uk:8080/doi/INVESTIGATION/24073300</a>



Epubs Expression Page

Some remarks on the analysis of the decay density matrix of mixed scalar-vector-tensor boson systems

HTTP URI - <http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1>



Publication Title	Nucl Phys B
Contributor	R.L Sekulin
Year	1973
Volume	56
Start Page	227
ISSN	05503213
BibCitation	R.L Sekulin, Some remarks on the analysis of the decay density matrix of n systems, Nucl Phys B 56 227 (1973)
Webtracks Ping	<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1/links">http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1/links</a>

http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1

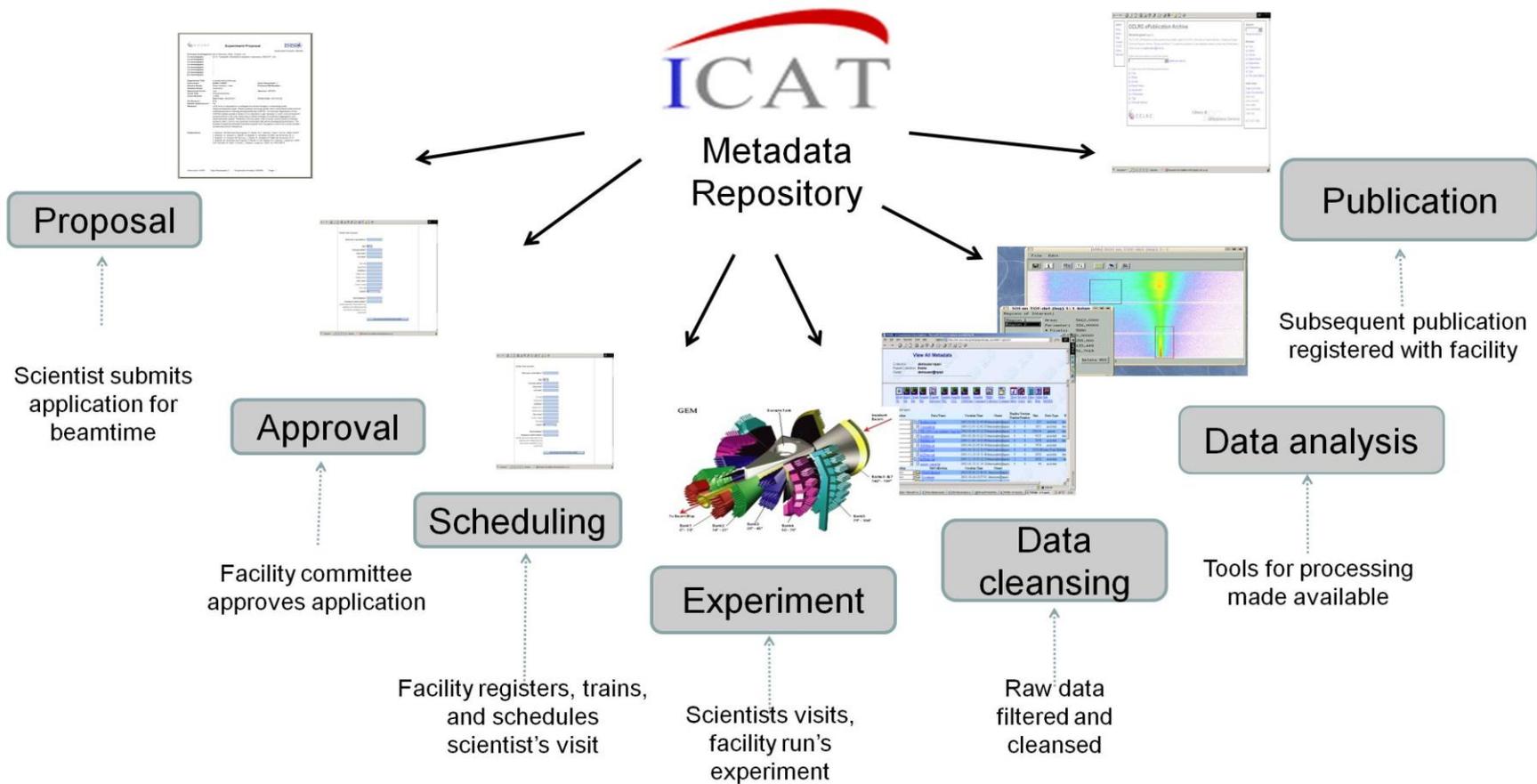
Citation links

Subject Resource URI	Property	Object Resource URI
<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1">http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1</a>	<a href="http://purl.org/spar/usesDataFrom">http://purl.org/spar/usesDataFrom</a>	<a href="http://tiger.dl.ac.uk:8080/doi/INVESTIGATION/24080016">http://tiger.dl.ac.uk:8080/doi/INVESTIGATION/24080016</a>
<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1">http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1</a>	<a href="http://purl.org/spar/cito/cites">http://purl.org/spar/cito/cites</a>	<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/23479/v/1">http://tiger.dl.ac.uk:8080/webtracks/expression/23479/v/1</a>
<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/21612/v/1">http://tiger.dl.ac.uk:8080/webtracks/expression/21612/v/1</a>	<a href="http://purl.org/spar/cito/isCitedBy">http://purl.org/spar/cito/isCitedBy</a>	<a href="http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1">http://tiger.dl.ac.uk:8080/webtracks/expression/56580/v/1</a>

Epubs Expression Links Page

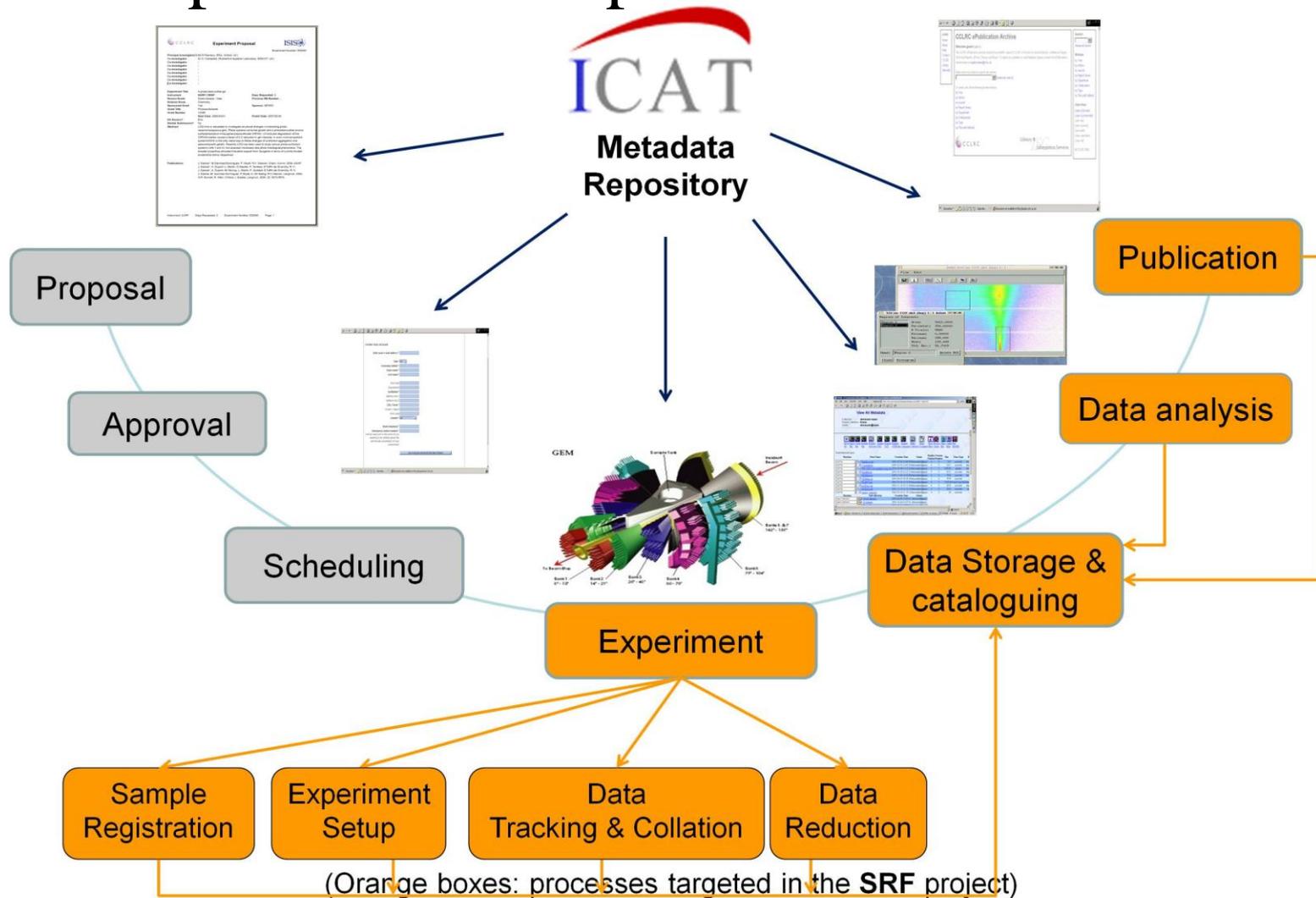
# Smart Research Framework

- experiments and the research life cycle



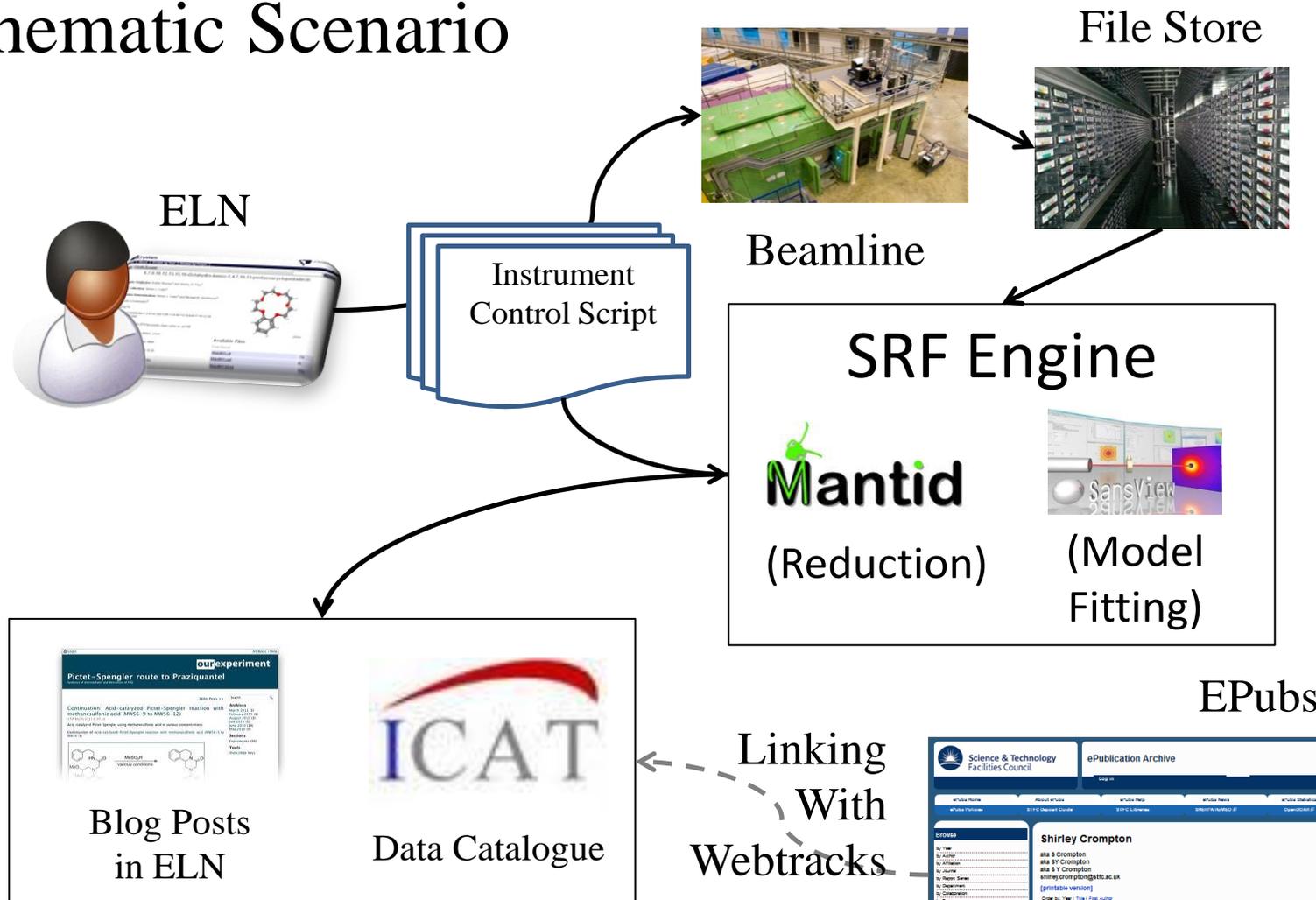
# Smart Research Framework

- in process provenance capture



# Smart Research Framework

## - Schematic Scenario



# Smart Research Framework

- blog posts capturing lifecycle events in an experiment

Current user: SRFUser | Log Out      Admin | All Blogs | Help | Support | About

## SANS2D Reduced Data

### SANS2D Complete Experiment

A blog mock up showing a complete SANS2D experiment

Older Posts >>>      Search

**Paper Published**  
16th August 2012 @ 14:38  
A paper has been published for the Amphiphiles for Supercritical CO2 experiment.  
View Paper  
SRFUser | Edit Post | RB43871 | Comments (0)

**Experiment Report Received**  
16th August 2012 @ 14:34  
An experiment report has been received for the Amphiphiles for Supercritical CO2 experiment.  
SRFUser | Edit Post | RB43871 | Comments (0)

**Anionic Surfactants and Surfactant Ionic Liquids**  
16th August 2012 @ 14:31

**Sansrun: 0120.xml**  
**RPA-Trimer-D2O\_SANS Experiment Details**

"test" code:	
Facility:	ISIS
Instrument:	SANS2D
User:	hqe71687
RB Number:	10372601
Title:	RPA-Trimer-D2O_SANS

**Input files**

"test" code:	
Sans Run:	00010320.nxs
Sans Trans:	00010309.nxs
Background Run:	00010311.nxs
Background Trans:	00010318.nxs
Direct Beam:	00010308.nxs
Path:	//130.246.36.41/ndxeans2d#/Instrument/data/cycle_11_4

**This Blog**  
New Post  
Blog Settings  
Timeline View  
Exhibit View  
Export Blog

**Archives**  
August 2012 (8)

**Authors**  
SRFUser (8)

**Sections**  
RB43871 (8)

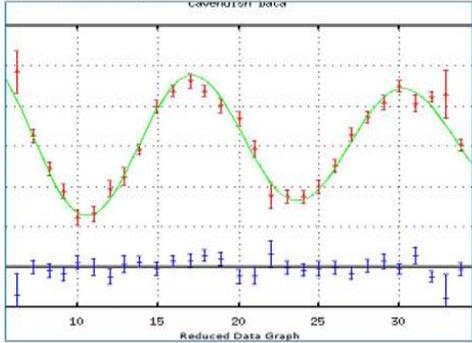
**Sansrun**  
0120.xml (1)

**Tools**  
Show/Hide Keys

### Instrument Parameters

"test" code:	
Monitors:	12.117

### Reduced Data Graph



SRFUser | Edit Post | RB43871 | Comments (0)

### Experiment Run Complete

16th August 2012 @ 14:29  
The Amphiphiles for Supercritical CO2 experiment run on SANS2D is now complete. Reduced data will be available shortly.  
SRFUser | Edit Post | RB43871 | Comments (0)

### Samples Registered

16th August 2012 @ 10:15  
Samples for the Amphiphiles for Supercritical CO2 experiment have been successfully registered.

**Summary:**  
10 Samples  
10 Background Samples  
1 Mask File

"test" code:	
RB Number:	RB43871

SRFUser | Edit Post | RB43871 | Comments (0)

Older Posts >>>

# Summary

## Collaborative Information Management via the intelligent pushing of citation links

- Leverage emerging Linked Data environment
- Link diverse types of digital research objects
- Facilitate access and discovery of related objects
- Restore context to dispersed digital research outputs
- No constraints on link semantics and metadata
- P2P, does not rely on a centralised service
- Flexible usage, link can be propagated at any time
- Mix and match research object networks from aggregated citation links according to the link resource/s or property/ies of interest.

• ....



Webtracks :

<http://www.jisc.ac.uk/whatwedo/programmes/mrd/clip/webtracks.aspx>

SRF : <http://www.mylabnotebook.ac.uk/>

Webtracks Download:

<http://sourceforge.net/projects/webtracks/files/>