



THE UNIVERSITY
OF QUEENSLAND
AUSTRALIA

The SCOPE System Scientific Compound Object Publishing and Editing

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The University of Qld
Australia

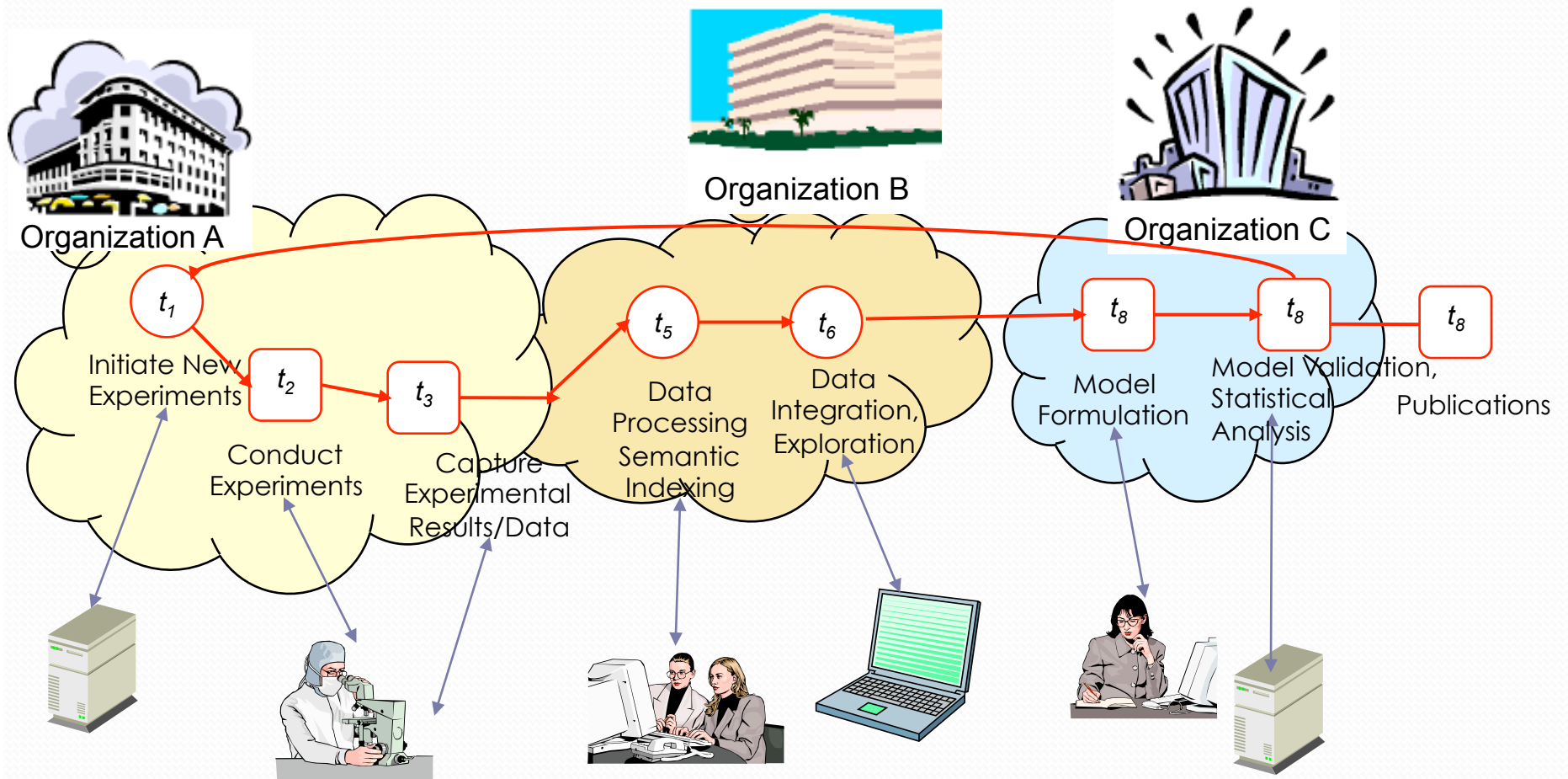
ORE, March 3, 2008

Scientific Publishing

Researchers are under increasing pressure to:

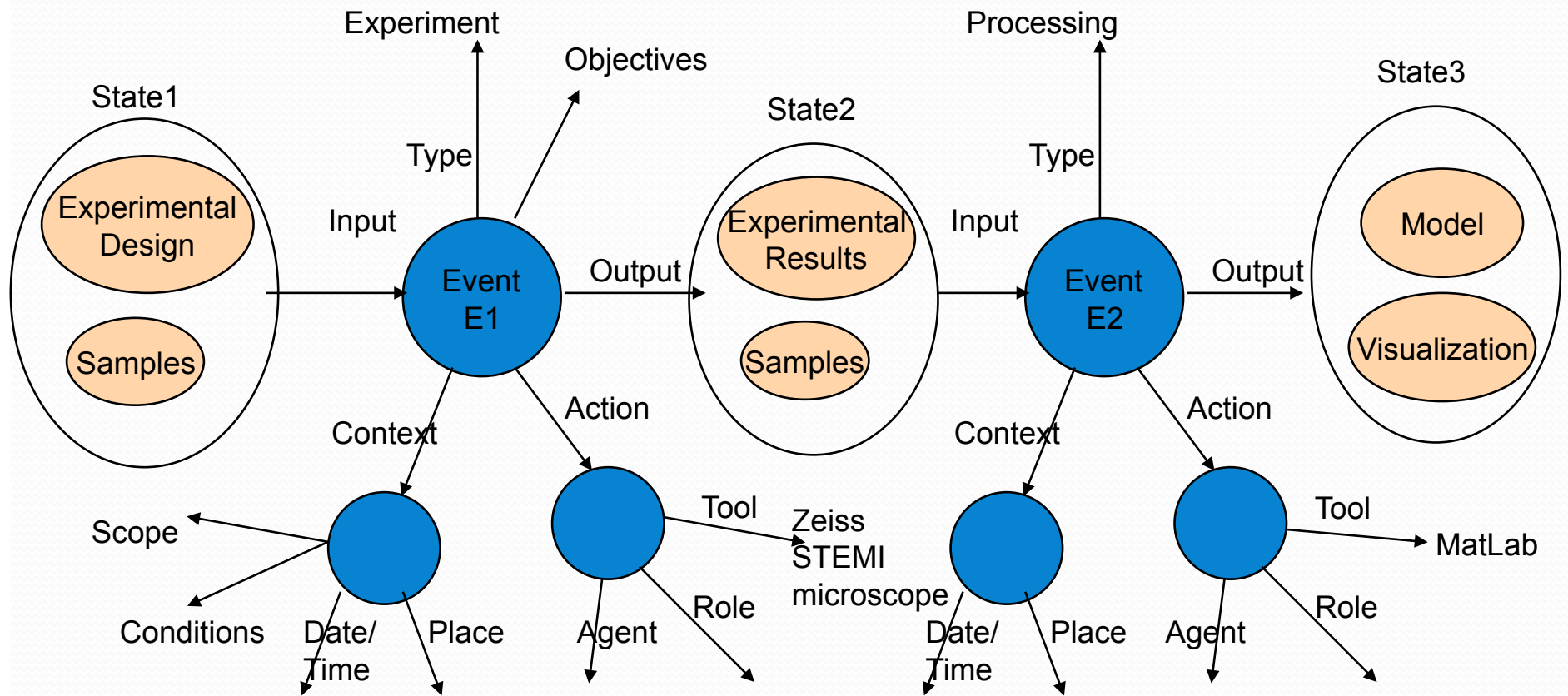
- publish raw and derivative data
- document precise provenance
- share data, methodology + analytical & modelling services
- enable review, re-use, repeatability and validation
- maintain competitiveness and protect IP

eScience Workflows



Kepler, Taverna, CombeChem, eLab notebooks
BPEL4WS – workflow based on web services

Modelling eScience Provenance -> RDF



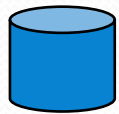
- Agents/Actors can be people, instruments or software e.g., web services
- Need to record events in both digital and physical world

Ideal - Scientific Publication Packages

	Area	Mean	S.D.	X	Y	Mode	Length	Major	Minor	Angle	Int.Der	Back.	Min	Max
1	0.01	208.2	88.14	0.34	0.06	253	0.34	0.11	0.08	102.7	0	0	35	253
2	0.01	206.8	89.14	0.17	0.07	253	0.34	0.1	0.08	17.57	0	0	35	253
3	0.01	212.9	84.54	0.26	0.11	253	0.37	0.11	0.1	158	0	0	35	253
4	0	190.4	98.85	0.07	0.1	253	0.21	0.07	0.05	76.53	0	0	35	253
5	0.03	228.8	68.54	0.67	0.38	253	0.75	0.24	0.15	154.8	0	0	35	253
6	0.09	240.7	50.36	0.34	0.48	253	1.24	0.38	0.3	95.89	0	0	35	253
7	0.08	240.1	51.46	0.59	0.59	253	1.18	0.35	0.28	81.38	0	0	35	253

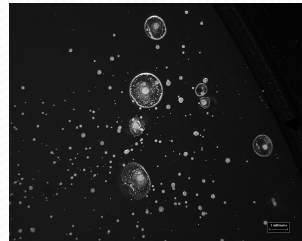
RDF
Package

External
Database

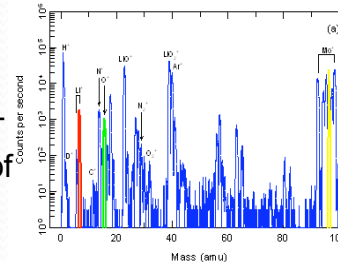


refers_to

Derived_from



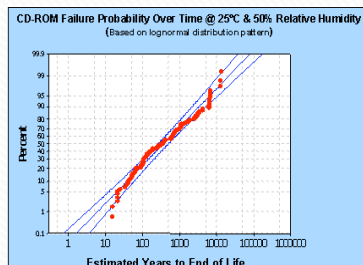
analysis_of



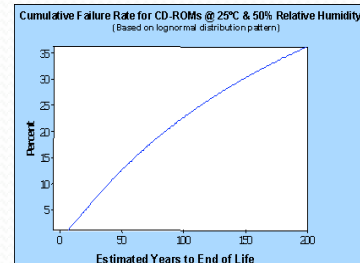
graph_of

$$\text{Average LE} = 1/T \exp -(A - B/T)$$

derived_from



refers_to



Slattery, O., Lu, R., Zheng, J., Byers, F., Tang, X.

"Stability Comparison of Recordable Optical Discs- A study of error rates in harsh conditions," Journal of Research of the NIST, 109, 517-524, 2004

Title
Creator
Description
Type
Discipline
Date.Published
License

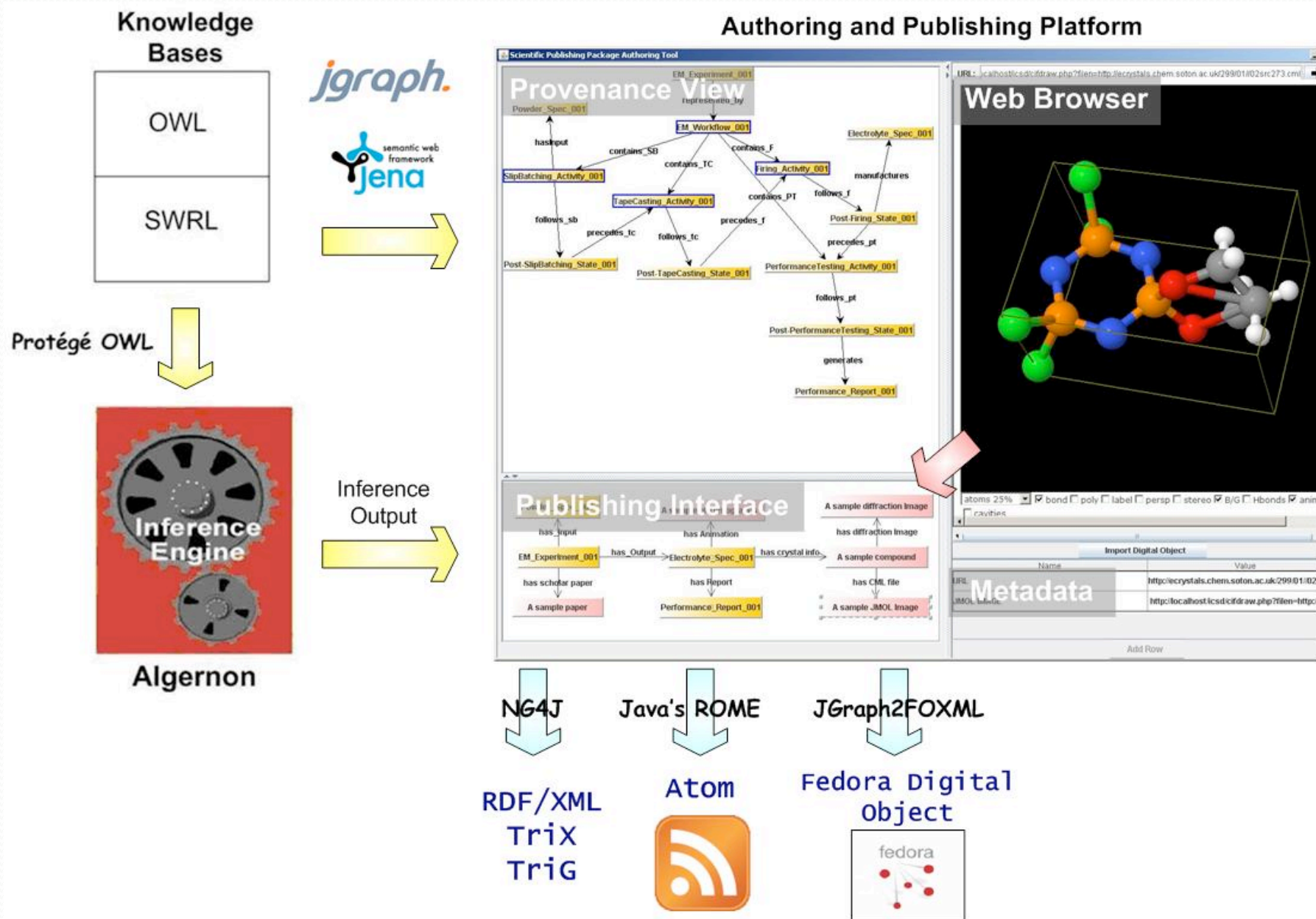
Each component has software, OS, hardware dependencies + interdependencies

Objective

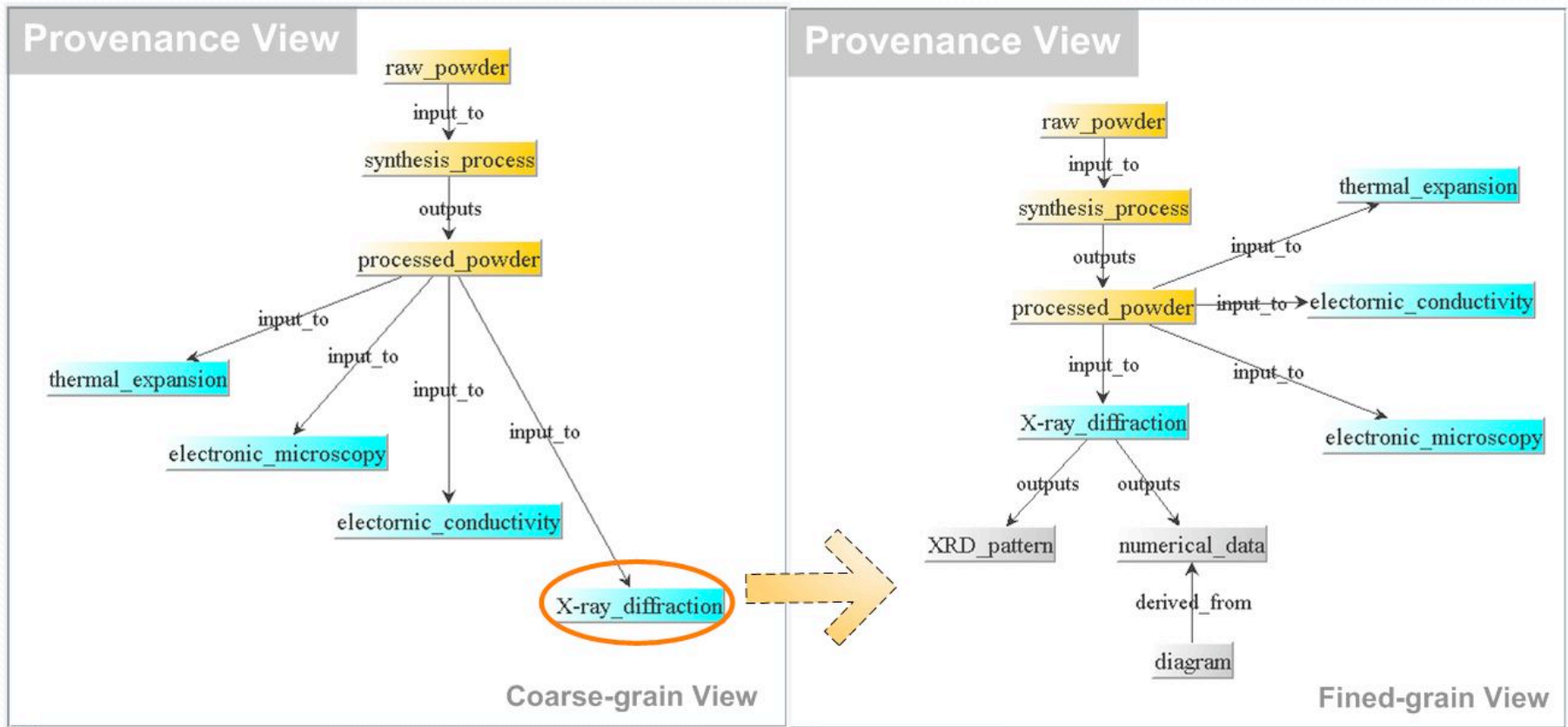
- Simple easy-to-use streamlined tool for authoring compound objects (OAI-ORE compliant)
- Interactive GUI to specify and link components retrieved from:
 - Web – institutional repositories
 - Visualized Provenance/Workflows - LIMS
- Label/infer relationships – with *type*
- Assign URI, attach metadata, license and publish
- RSS notification



Architecture



Provenance Explorer

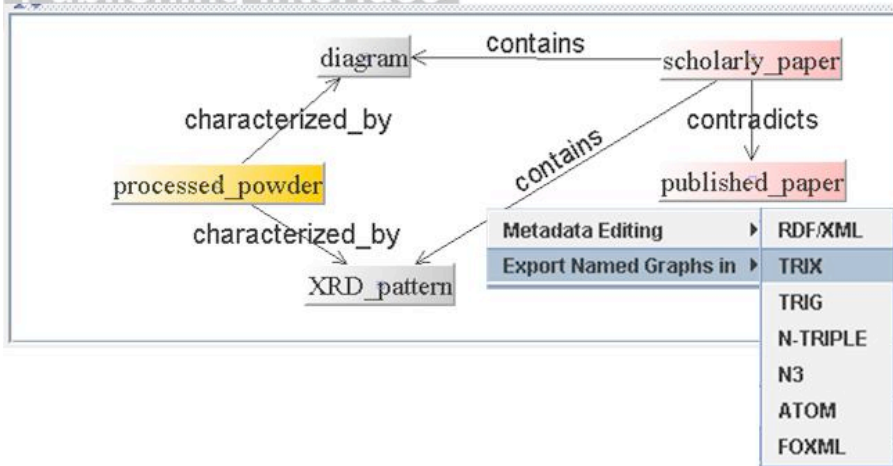


Publishing Process

1. Assign URI, and update/enhance Metadata for Compound Object
2. Attach Creative Common License
3. Publish as:
 - RDF/XML
 - TriX , TriG, N-Triple, N3
 - Atom
 - FOXML
4. Ingest to Fedora

Export Named Graph in TriX

Publishing Interface



Named Graphs in TriX

```
OAI-ORE Scientific Compound Object.trix - Notepad
File Edit Format View Help

<triple>
  <uri>http://localhost/oai-ore/A_Novel_Metal_Oxide_for_SOFC</uri>
  <uri>fedora:hasPart</uri>
  <uri>http://localhost/oai-ore/processed_powder</uri>
</triple>
<triple>
  <uri>http://localhost/oai-ore/processed_powder</uri>
  <uri>http://localhost/oai-ore/characterized_by</uri>
  <uri>http://localhost/oai-ore/XRD_pattern</uri>
</triple>
<triple>
  <uri>http://localhost/oai-ore/scholarly_paper</uri>
  <uri>http://localhost/oai-ore/contains</uri>
  <uri>http://localhost/oai-ore/XRD_pattern</uri>
</triple>
.....
....
```

Output as Atom

Publishing Interface

```
graph TD; processed_powder -- characterized_by --> diagram; processed_powder -- characterized_by --> XRD_pattern; diagram -- contains --> scholarly_paper; XRD_pattern -- contains --> scholarly_paper; scholarly_paper -- contradicts --> published_paper;
```

Metadata Editing

Export Named Graphs in

- RDF/XML
- TRIX
- TRIG
- N-TRIPLE
- N3
- ATOM**
- FOXML

The Atom Feed

A Novel Metal Oxide for SOFC

You are viewing a feed that contains frequently updated items. Items from the feed are automatically downloaded to your computer.

Subscribe to this feed

Scholarly Paper

Sunday, 12 August 2007, 11:30:31 AM | Smith, John →

Published Paper

Sunday, 12 August 2007, 11:30:31 AM | M. A. Tena, et al →

XRD Pattern

Sunday, 12 August 2007, 11:30:26 AM | Dr. Janet GoodChild →

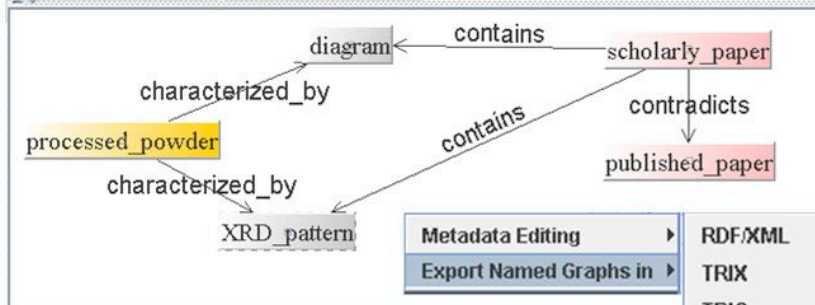
Processed Powder

Sunday, 12 August 2007, 11:30:21 AM | Dr. John Smith →



Output as FOXML

Publishing Interface



Fedora Digital Object

fedora

Fedora Digital Object

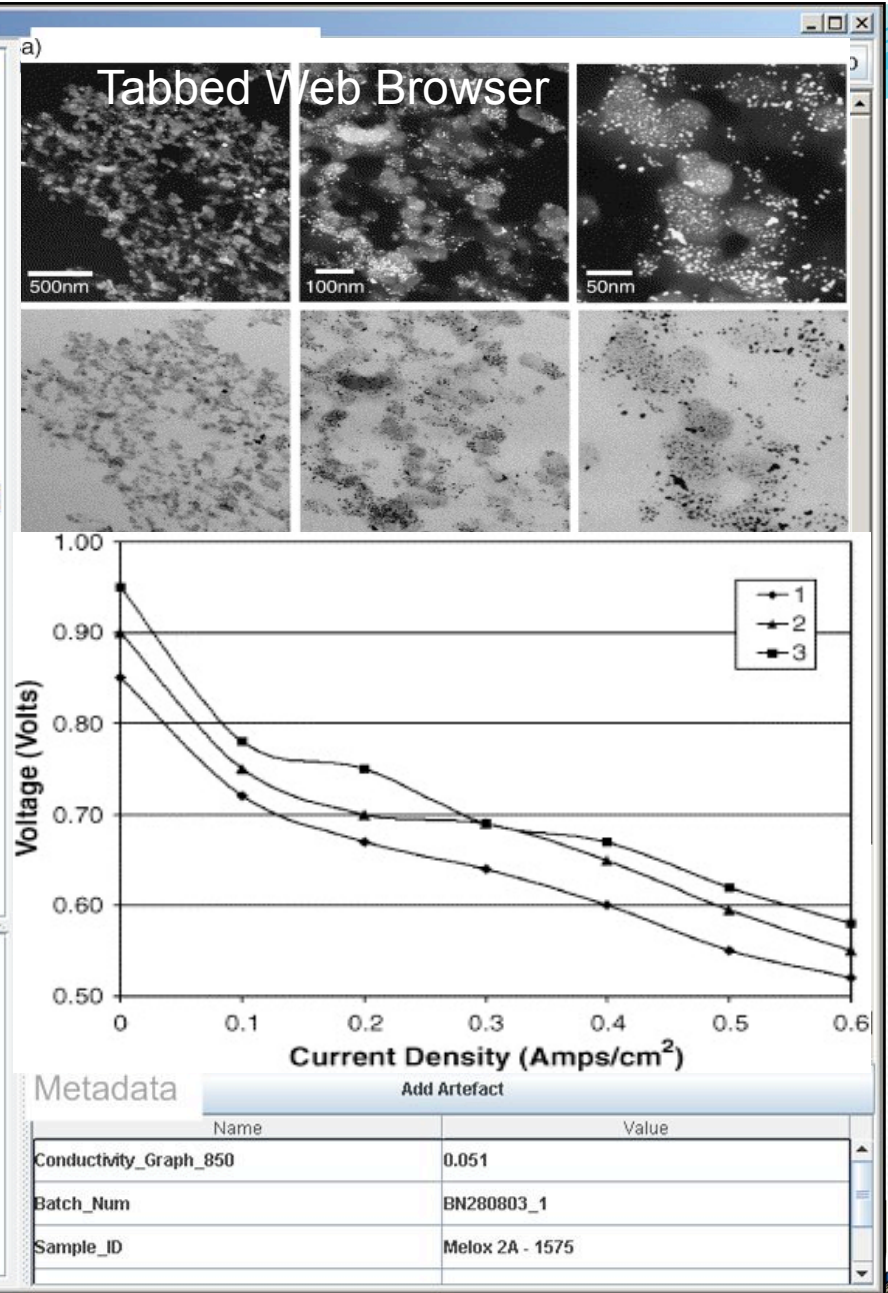
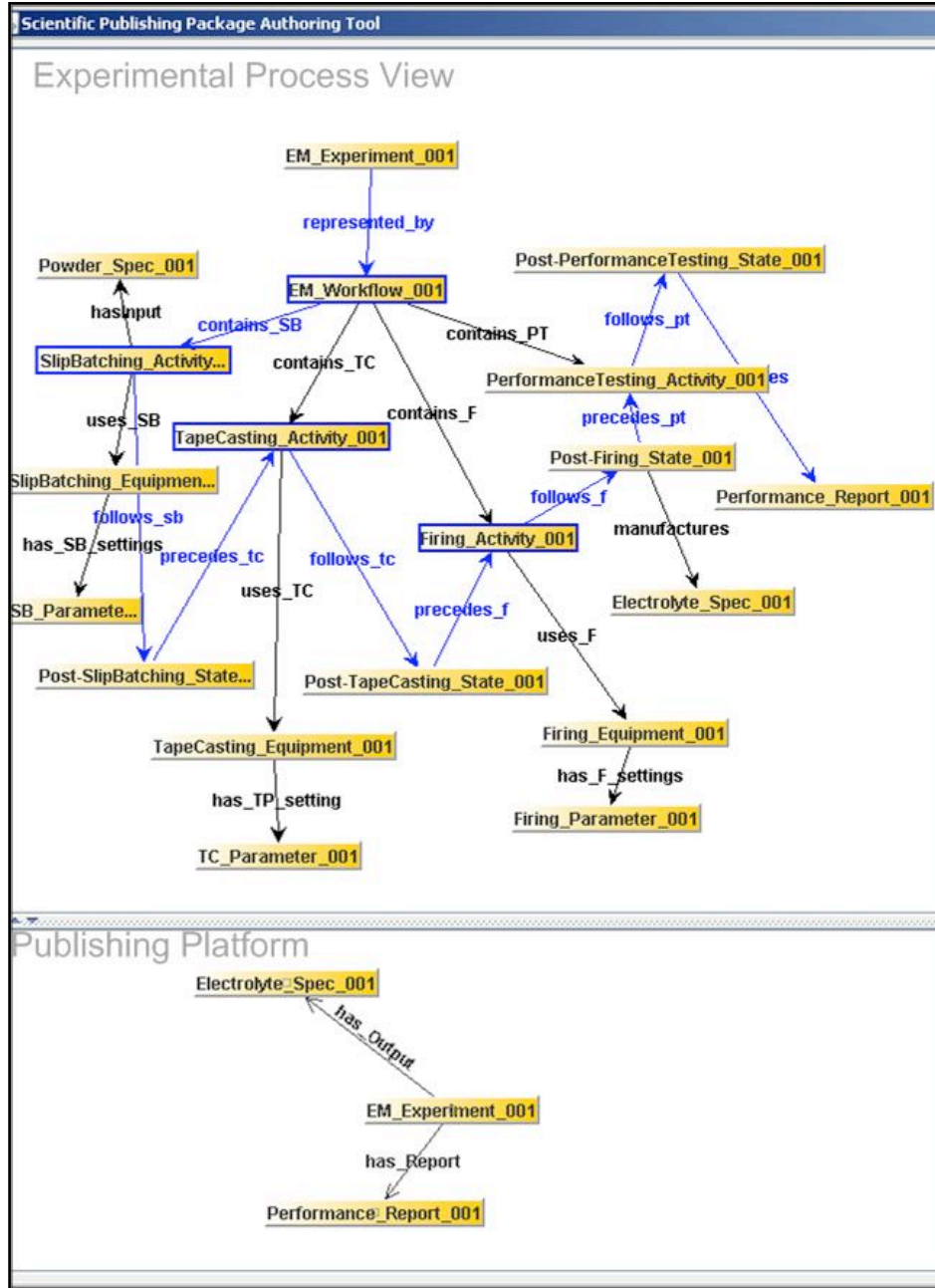
Default Disseminator - Item Index View

Object Identifier (PID): **demo:OAI_ORE_ScientificCompoundObject**

Version Date: current

Item ID	Item Description	MIME Type
DC	Default Dublin Core Record	text/xml
RELS-INT	Component to Component Relationship in RDF	text/xml
Scientific_Object_Representation	A Novel Metal Oxide for Enhancing Conductivity in Solid Oxide Fuel Cell	text/html
RELS-EXT	Composite Relationship in RDF	text/xml





Compound Object Display


Vannotea2006

File Edit Help

Media Browser

Free Content Related

Address <http://maenad.itee.uq.edu>



X-Ray diffraction data that, when processed, produces 3D crystal structures of proteins.

CCD frames from Bruker SMART 6000 CCD detector

Streaming video from JCU Lab

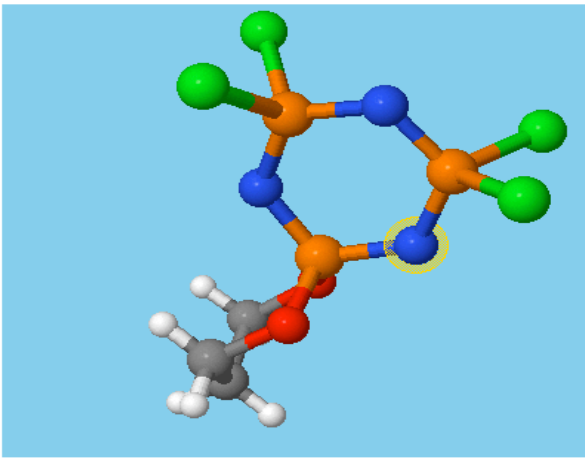
3D Rotation of processed crystal (RSCB view)

3D Rotation of processed crystal (atoms)

[Back to Media Files Index](#)

model.cif

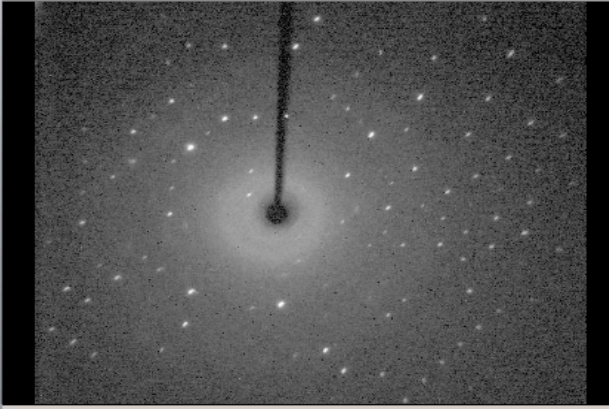
<http://maenad.itee.uq.edu.au/imrank/crystallography/cyclophosphazene/mo>



Context: //N3//number:12,moveto//1//127//520//845//75.3//156

compedshot3.mov

<http://maenad.itee.uq.edu.au/imrank/crystallography/cyclophosphazene/ima>



Paused 0 00:00:00 00:02:39

<http://ecrystals.chem.soton.ac.uk/299/>

<http://ecrystals.chem.soton.ac.uk/299/>

Address <http://ecrystals.chem.soton.ac.uk/299/>

(6,7)10-15(9-13)11-2-1-3-12-15/h8-10,13-15H,1-3H2

Compound Class: Inorganic
Keywords: cyclophosphazene, phase transition, variable temperature
Creation Date: 28 March 2007
Deposited By: Dr Simon J Coles
Deposited On: 28 March 2007
Data collection parameters

02src273.cif	12k
02src273.cml	4k
Validation	
02src273_checkcif.htm	8k
Refinement	

Done

Jabber Client

Disconnect Connect Enter Conference Leave Conference

Conference Room (drag&drop users to invite them)

- exodus2
- imrank
- mjh (Logged out)
- ronalds

Connected

Annotea Timeline Jabber Client Record and Replay Jabber Chat

For Further Information

<http://www.openarchives.org/ore/>

<http://www.itee.uq.edu.au/~ereseach>

Contacts: j.hunter@uq.edu.au

kwokc@itee.uq.edu.au

DCC, Dec 12-13, 2007



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