

A BioCatalogue

Cataloguing Web Services for the Life Science Community

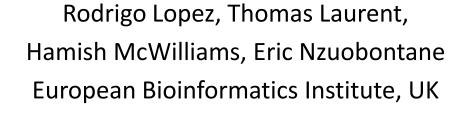
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David De Roure, myExperiment



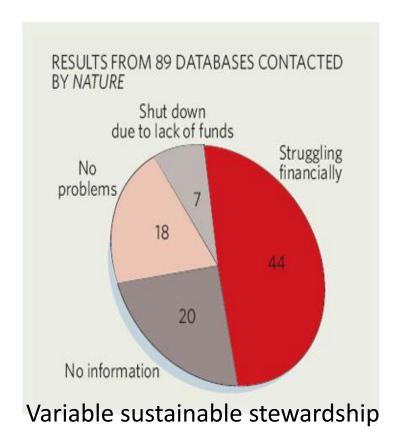
Web Services in the Life Sciences

- Programmatic Interfaces to services on the rise
- EMBL-European Bioinformatics Institute
 - 3 million/month accesses to Web Service APIs
 - 1 million/month compute jobs > 50% are over WS
- Guessimate 1000-1500 services.
- Why?
 - Specialisation and segregation of methods from monolithic servers.
 - How one should publish data.
 - Automated Life Science applications, like workflow systems Taverna, Kepler, Triana, Trident, KNIME, BPEL



Chain stores and Boutiques

- Major data centres and national centres
 - EMBL-EBI (UK), DDBJ, PDBJ (Japan), NCBI, SDSC PDB (USA)
- Investigator and community projects



- Kanehisa Laboratory, Kyoto, Japan
- BASIS, University of Newcastle, UK
- Biomolecular Interaction Network Database, BIND, University of Toronto, Canada
- Institute of Bioinformatics, Tsinghua University, China
- EMAP, Edinburgh Mouse Atlas Project, UK
- The Chemical Informatics and Cyberinfrastructure Collaboratory (CICC), Indiana University, USA

and more and more....



Service Flavours

- Generalist
 - SOAP
 - REST

- Specialist
 - DAS (Distributed Annotation Services)

www.biodas.org

- BioMOBY

www.biomoby.org





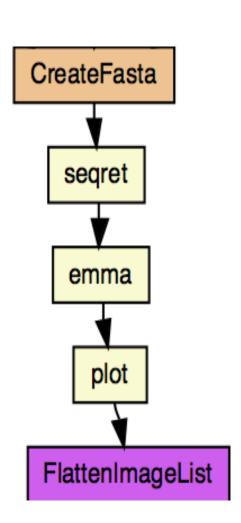
Web Services in the Wild

Visible? Findable?

- "EMMA" is the Clustalw multiple sequence alignment program from the Emboss suite
- Poor adoption for providers.
- Forum for advertising and shopping.

Executable?

- WSDL, WADL, WSDL2, Other kinds of services.
- Transcend the specific grounding





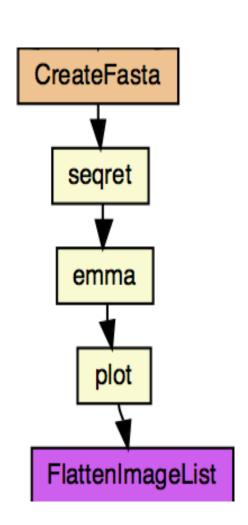
Web Services in the Wild

Understandable?

- Input0:string, Output0: string?
- What does the SeqRet actually do?
- Examples? Example data? Example Parameter configurations? Input-Output correlations?
- Adequate documentation for anonymous reuse.

Usable? Available?

- Quality of Service, robustness, test scripts?
- Stability and dependability (see BioMART)?
- Licensing, execution restrictions?
- Trust and risk.
- Monitoring and intelligence gathering.





Cataloguing Services

- Investigator and project specific registries
 - EMBRACE, BioSapien, Stargate Portal
- Community lists
 - Bioinformatics Links Directory, BioLinks,
 BioPlanet,
- Project specialist registries
 - BioMOBY Central, DAS Registry, myGrid Registry, Sswap
- General catalogues and search engines
 - SeekDa!, Web Services List, XMethods

Sustainability and curation

Accessibility

Rich annotation & customisation

Provider engagement



Lets Pool our Knowledge

- A reliable, trusted, up to date and sustained catalogue customised for the Life Sciences.
 - EBI curation and service commitment
- Discovery interface for decision support.
 - Drawing on myExperiment and EBI legacies
- Community and specialist curation.
 - Pooled and accumulative annotation.
 - A platform for service monitoring and analytics.
- Incorporated into applications and mashups.
 - Itself a web service, with a (REST) API.



BioCatalogue: providing a curated catalogue of Life Science Web Services.



BioCatalogue will provide a single registration point for Web Service providers and a single search site for scientists and developers.

BioCatalogue will also act as a place where the community can find contacts and meet the experts and maintainers of these services.

Started June 08 Closed pilot Dec 08 Pilot release April 09



BioCatalogue-Friends focus group Perpetual beta

Three year award

"Web Services are hard to find..."

SEARCH

Scientist, tool developers, bioinformaticians will be able to find the right Web Service they were looking for, thanks to an easy and powerful search interface harvesting the information made available by the Web Services providers and the BioCatalogue community.

"My Web Services are not visible..."

REGISTER

Service providers will be able to easily register their Web Services in the BioCatalogue, making them instantly available to the scientific community as well as the tool developers.

"Web Services are poorly described..."

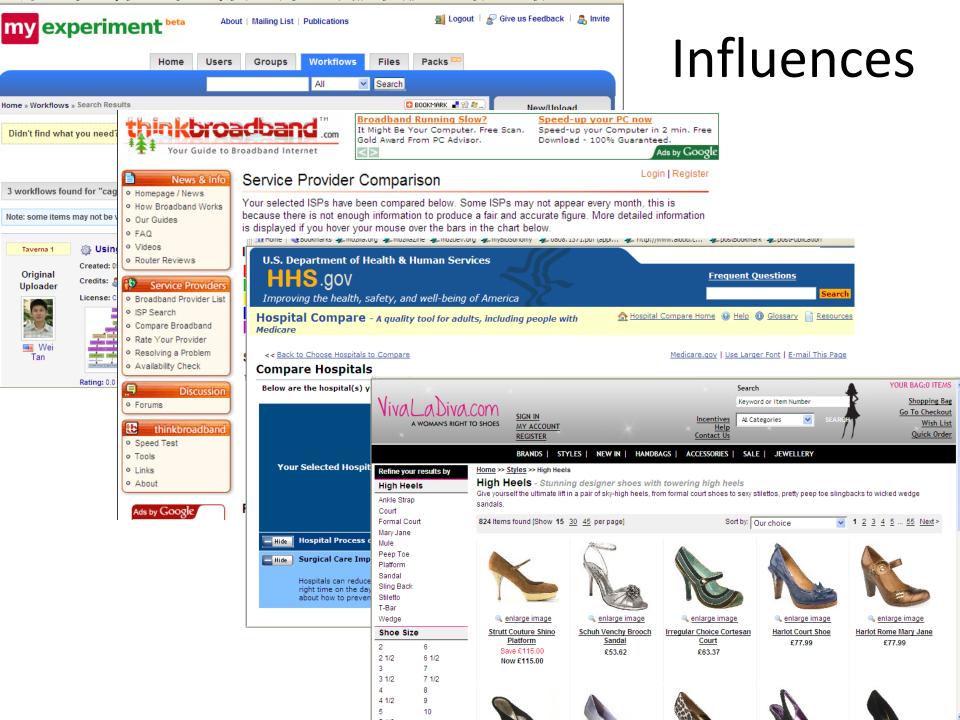
ANNOTATE

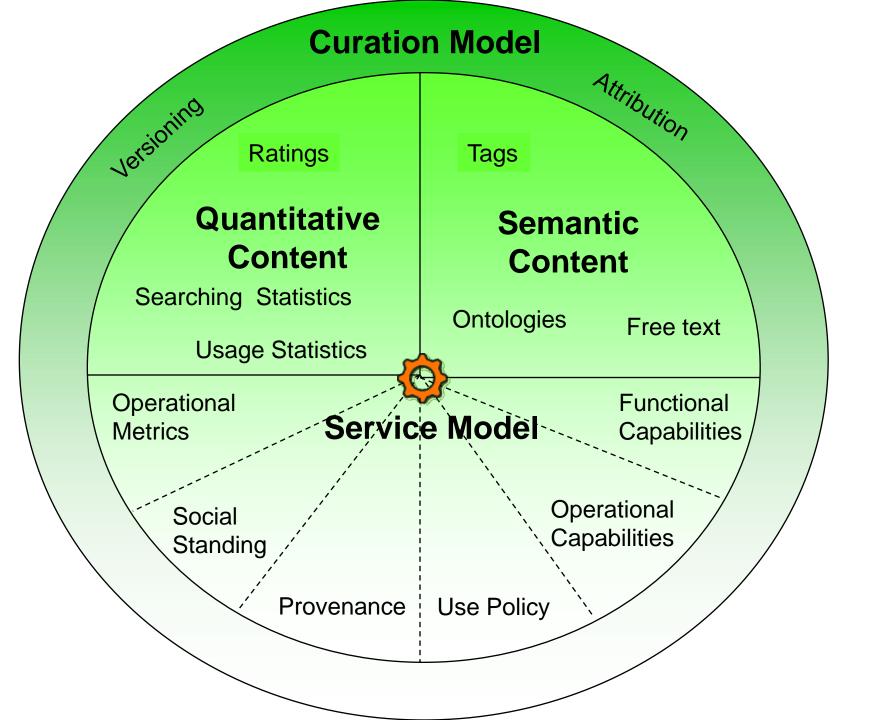
Expert curators will provide oversight, monitor the catalogue and provide high quality annotations for services. The wider community will also participate to this effort using social networking for recommending, tagging, commenting and rating the services.

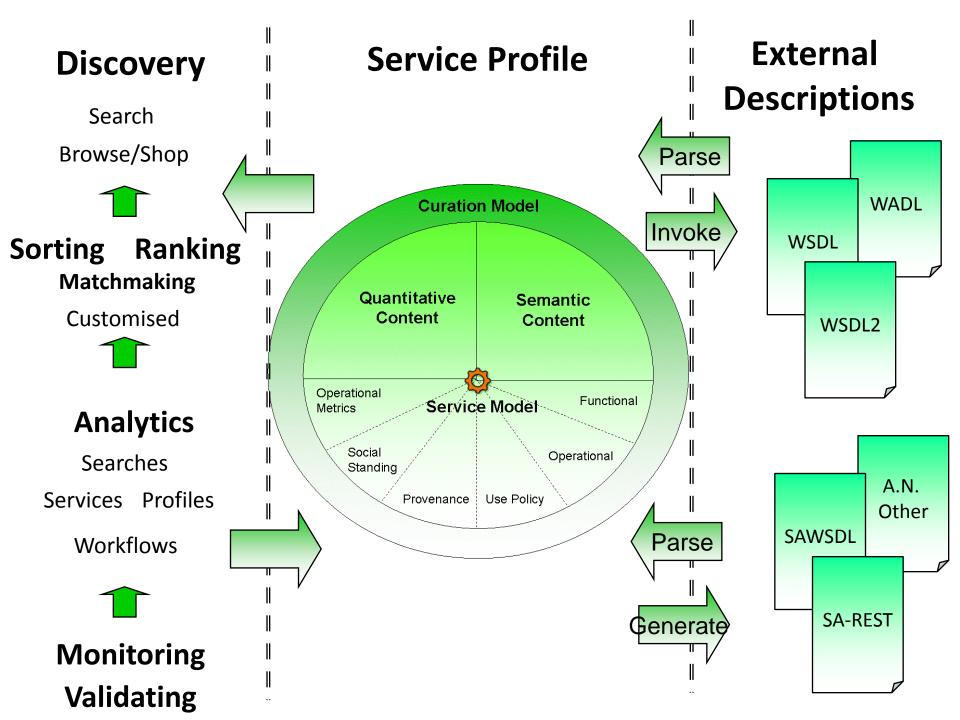
"Web Services are volatile..."

Web Services are volatile. They change their location, capability and interaction or become outdated. BioCatalogue will allow agents to monitor the Web Services and automatically add information to the catalogue.

the University of Manchester and the EMBL-EBI. the BBSRC (BB/F01046X/1, BB/F010540/1)

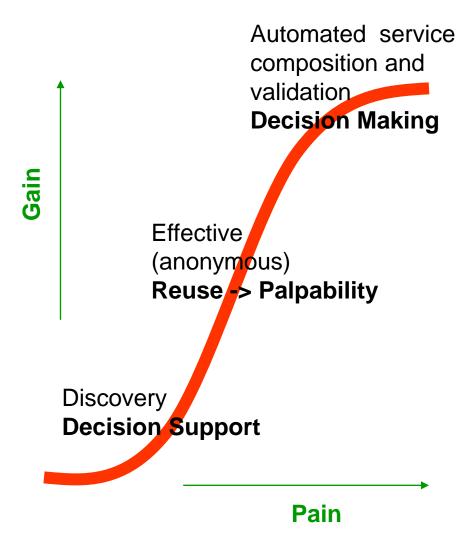








Modelling Functional Capability



- WSMO http://www.wsmo.org
- OWL-S http://www.w3.org/Submission/OWL-S
- SAWSDL http://www.w3.org/2002/ws/sawsdl/
-
- Tags
- Ontology
- myGrid Service Ontology
- Text Descriptions

[Lord et al 2004]



myGrid Functional Capability Ontology

Service

Operations

Inputs

Outputs

Task

Method

Resource

Domain Content Service features Grounding **WSDL**

Informatics

Bioinformatics

Molecular Biology

Formats

Tasks

W3C OWL and RDFS
Number of classes ~750
myGrid and BioMOBY



Free text and tagging in the user's language

Smart interfaces for people

Semantically annotated services for driving interfaces and automated processing



People-Powered Registration

- By Provider and by Proxy.
- Ownership.
- Incentives
- Completeness vs Cost.
- Relative rankings feedback.
- Visibility and reputation.
 (which may not always be flattering)
- Do not presume that providers are unhelpful.





People-Powered Curation

- Third party and Provider
- Curation@Source/Delivery
- Incentives.
 - Quick and easy.
 - Credit (and Blame).
- Incremental and partial descriptions.
- Peer review. The Wisdom of the Wisdom of the Crowd
 - Quality, Slander
- Content.



Distributed Human Grid of Annotators. Annotation Jamborees. T Shirts.



Expert Curation

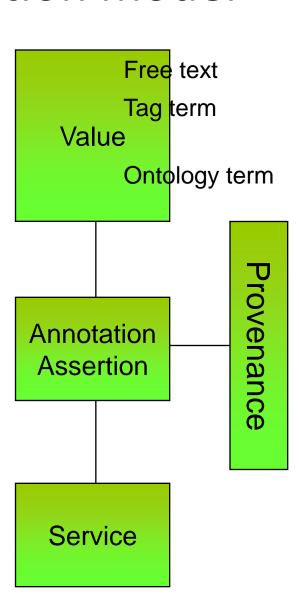
- Added value of Biocatalogue
 - Review
 - Quality assurance and Trust
- Enriched annotations
- A curation pipeline.
 - Tags to Ontologies.
 - Ontology husbandry
- A Sweatshop.
 - How do we make this smarter?





Uniform Annotation model

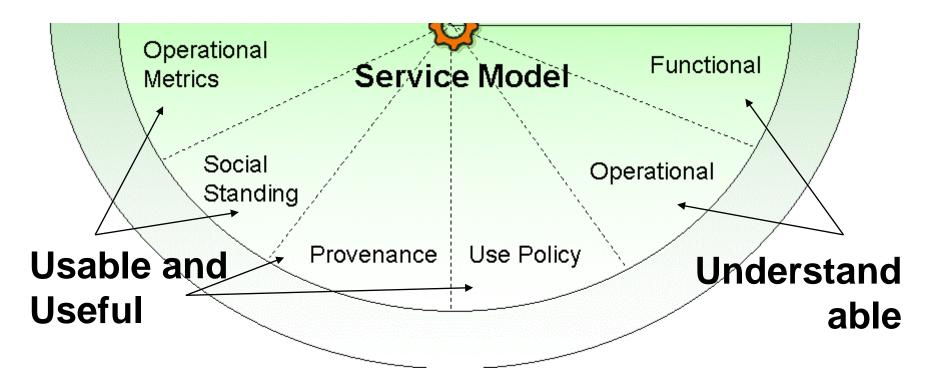
- Minimum for discovery and invocation
- Partial annotations
- Multiple annotations
- Polymorphic: text, tags, statistics, ontologies
- Annotation provenance
- Trust
- Curation pipeline and monitoring
- Multiple providers
- Multiple versions
- Multiple deployments

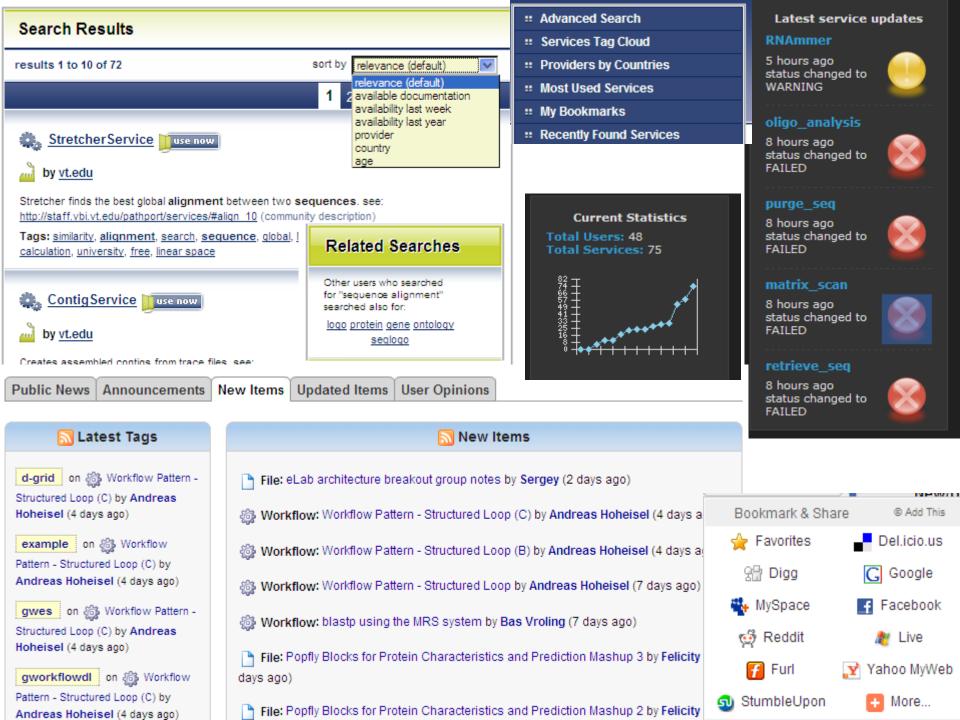




Ranking, Sorting, Filtering and Comparing

- Grading: bronze -> platinum
- Presence, quantity and quality
- Judgement by the users, not us.







Auto Curation



Auto scavenging

SeekDa!

Auto Annotation

- Specialist parsing
- Auto-tagging
- Text mining
- Inferring service descriptions from myExperiment workflows (Quasar framework)

Auto Monitoring

- Test Workflows / scripts
- Service monitoring
- Feeds from applications and third parties: dial home diagnostics, customer reports, predicted down times

Auto Usage Analytics

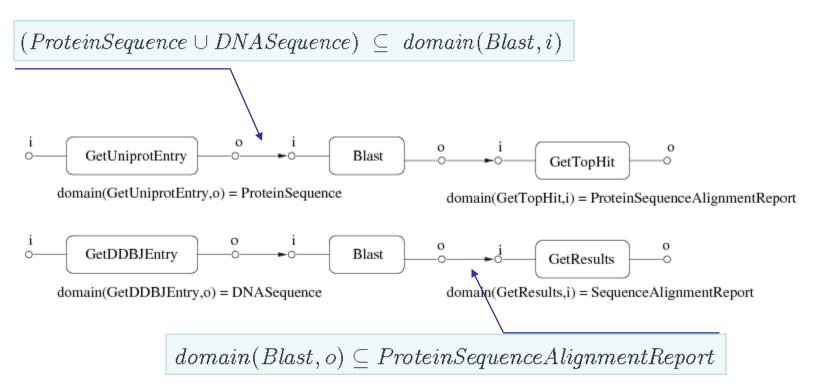
- Workflow usage
- Search patterns



Quasar

Quality Assurance of Semantic Annotations for Services

Using mismatch-free workflows to infer information about the semantics of linked parameters



Users	registration Identity management profile management ownership account management bookmarking notification
Services	soap services registration dashboard versions scavenging wsdl parsing instances Identity management
Discovery	text search browse and drill down usage-based tag search sorting on criteria and categories recommendations
Curation	tagging specialist parsers. ratings 500 services 250 full curated seeded controlled vocab. recommendations.
Monitoring	registration test scripts live tests QoS app feeds WsdI monitoring
Integration	REST API myExperiment Open Search
Content	Batch migration Policy identification Provider engagement



"The Life Science Web Services Registry"

Welcome jits L			
Search:	Go! Browse Register a Servi	ice	
New SOAP Service			
1. Specify the URL to the			
vww.ebi.ac.uk/Tools/webser	51 G ()	<u> </u>	
2. Check the details, then BioCatalogue			
After submission you will be	Dio Gatatogae		
After Submission you will be	"The Life Science Web Services Registry"		
1-6			
Information from	Search:	BioCatalogue 💮	
Name: WSWUBlastService		"The Life Science Web Services Registry"	
		The Life Science Web Scivices negistry	
WSDL Location:	Search Results	Search: Go! Browse Register a Service	
http://www.ebi.ac.	Search Results		
Description:	Search query: "blast"	Service: Blast SOAP	
Documentation for t	Search query: "blast"	Submitted by: jits (about 1 hour ago)	
Location:	Services (2)	Unique code: blast_927483	
United Kingdom			
		No description	
This service has the		Latest Version Endpoint(s):	
blastp (3 inputs, 1 o	Blast SOAP	http://xml.nig.ac.jp/xddbj/Blast	
blastn (3 inputs, 1 o getOutput (1 input,		All Location(s): Japan	
getXML (1 input, 1 c runWUBlast (2 input	No description		
checkStatus (1 input poll (2 inputs, 1 out	Provider(s): xml.nig.ac.jp	All Provider(s): xml.nig.ac.jp	
getResults (1 input,	Submitted by: <u>iits</u> (41 minutes ago)		
getIds (1 input, 1 or polljob (2 inputs, 1		WSDL Location: http://xml.nig.ac.jp/wsdl/Blast.wsdl	
doWUBlast (2 inputs	Blast Service SOAP	Operations (6):	

Name: searchParam

Blast @ IBCP (http://gbio-pbil.ibcp.fr)

SeekDa!

BioSapien myGrid

Feed

BioCatalogue The Life Science Web Services Registry

EMBRACE Migrate

Feed and Cross-link

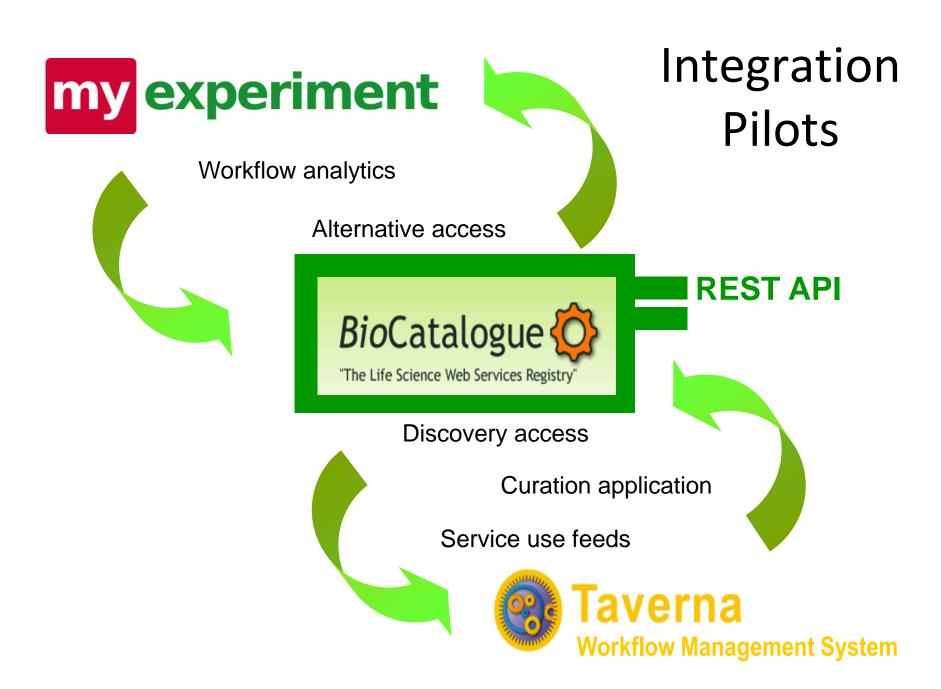
myExperiment Code Base

Scrape

BioMOBY Central

DAS Registry

BioLinks





So why is it taking so damn long to get here?

- The final 9 yards and 80:20 rule.
- All or nothing.
- Dedicated resources and best intentions.
- Content, content, content.
- Being too damn, and unnecessarily, clever.

A social activity



BioCatalogue Team



Hamish McWilliams



Rodrigo Lopez



Thomas Laurent



Mark Wilkinson





Franck Tanoh





Jiten Bhagat



Carole Goble





Further information

- http://www.biocatalogue.org
- Join our friends
- Supply technology!

Carole Goble, Robert Stevens, Duncan Hull, Katy
 Wolstencroft, Rodrigo Lopez, Data Curation + Process
 Curation = Data Integration + Science, Briefings in
 Bioinformatics, in press