Research Objects and WS Characterization

Jose Enrique Ruiz
jer@iaa.es

November 29th 2012
Workflows Group ASOV France

Wf4Ever

2011 - 2013

Advanced Workflow Preservation Technologies for Enhanced Science

1. Intelligent Software Compon… Spain)
2. University of Manchest…
3. Universidad Politécn… Spain)
4. Poznan Superco… King C…
5. University of… OXF, U…
6. Institut… lucía (…
7. Leiden U… dical C…

Reproducible Science

Web-services based Workflows

The University of Manchester

MANCHESTER 1824

POZNAN SUPERCOMPUTING NETWORKING

INSTITUTO de ASTROFISICA de ANDALUCIA CSIC I·A·A

iSOCO enabling the networked economy

LUMC

SEVENTH FRAMEWORK PROGRAMME

European Commission Information Society and Media

Astronomy Research Lifecycle

Astronomy research lifecycle is **entirely digital**

- Observation proposals 
- Data reduction pipelines
- Analysis of science ready data
- Catalogs of objects and data
- Publish process 

  - Final data results
  - Experiment in DL ADS/arXiv

Reproducible research is still not possible in a digital world

A normalized preservation of methodology is needed

Efficient use of rich data infrastructure (VO) may be improved

Tools

Efficiency and Reuse

Optimize return on investments made on big facilities

- Avoid duplication of efforts and reinvention
- How to discover and not duplicate ?
- How to re-use and not duplicate ?
- How to make use of best practices ?
- How to use the rich infrastructure of data ?
- **Intellectual contributions are encoded in soft**

More data in archives does not imply more knowledge

- Time has come to go beyond the PDF
- Expose complete scientific record, not the story
- Allow easy discovery of methods and tools

Barriers to Data and Code Sharing in Computational Science

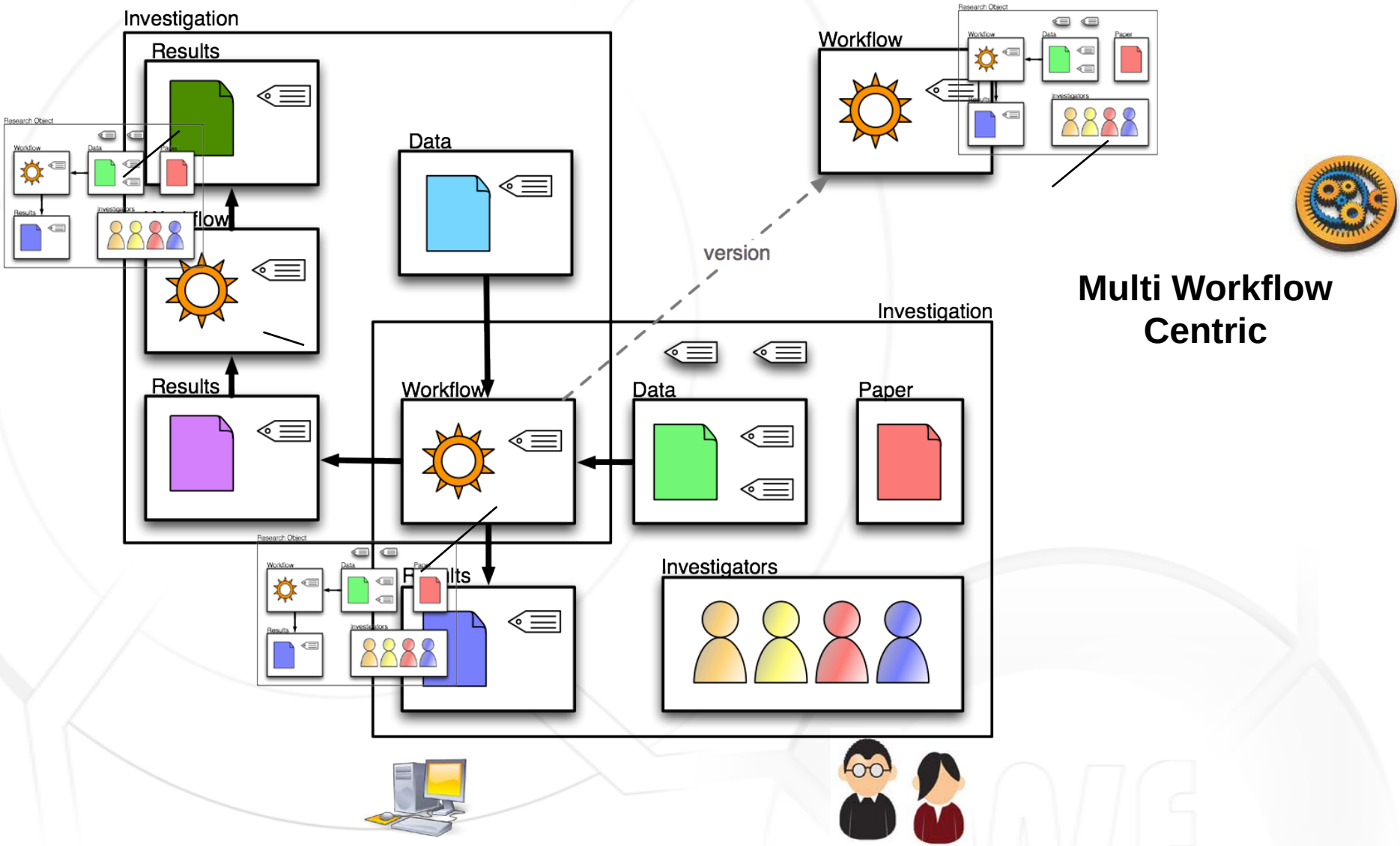
Survey of Machine Learning Community, NIPS (Stodden, 2010):

Code		Data
77%	Time to document and clean	54%
52%	Dealing with questions from users	34%
44%	Not receiving attribution	42%
40%	Possibility of patents	-
34%	Legal Barriers (ie. copyright)	41%
-	Time to verify release with admin	38%
30%	Potential loss of future publications	35%
30%	Competitors may get an advantage	33%
20%	Web/disk space limitations	29%

I don't know how

Tools

Research Objects in Wf4Ever



RO Content

- Process (workflows), data, external resources and bibliography
- Execution environment set-up and local software dependencies
- Experimental protocol followed
- Roles, types and relationships among all digital components
- Provenance of intermediate and final results
- Decomposable attribution and authoring
- Fine-grained access control and permissions
- Example datasets for demonstration, reproducibility, monitoring, etc

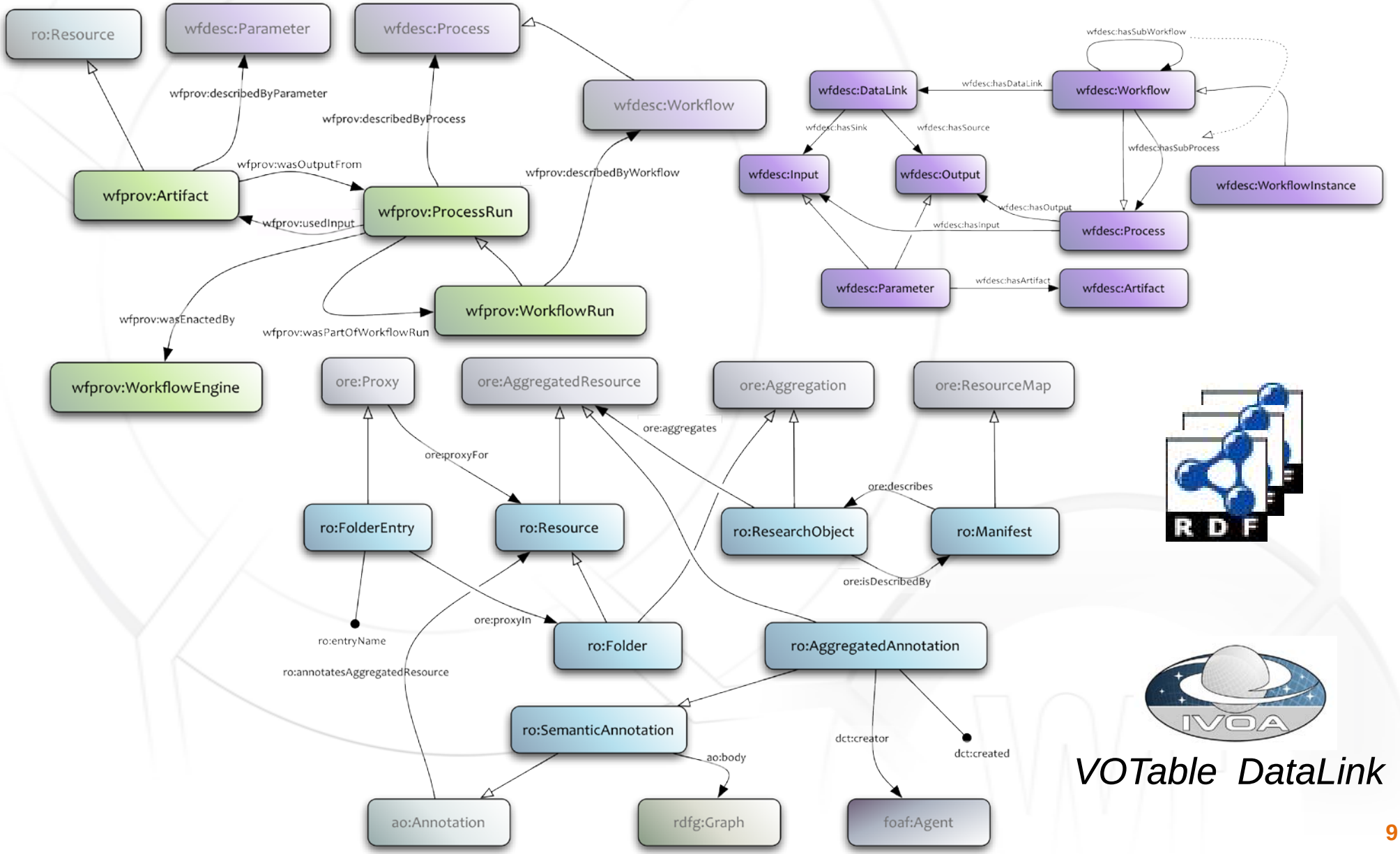
RO Template

- Placeholders to ease the aggregation process
- Completeness checking/quality assessment

Semantic Annotations

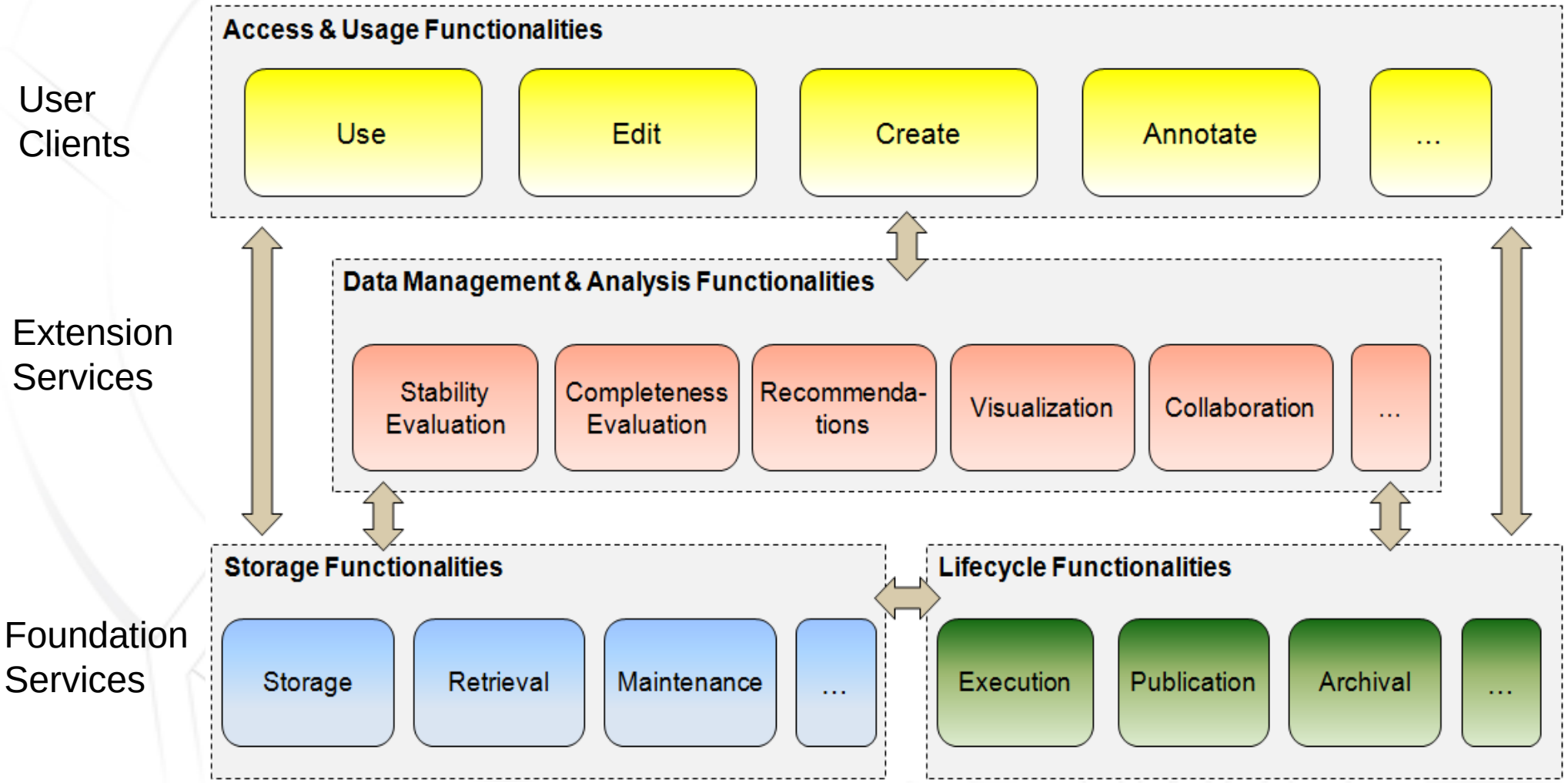
- Author of an **annotation**
- **Author and co-authors** of a **workflow**; reference link to a re-used workflow and its author
- Who has performed the **execution** of a workflow leading to the results provided in the RO
- Computing execution environment of the RO and local software **dependencies**
- Special **access requirements** to web services
- Datasets **provider**: person, webpage, survey, data release, etc.
- How much **time** does it take to run a workflow using the full data and the provided subsample
- The number of **elements** of the sample dataset where one workflow and/or RO iterates
- Previous and subsequent workflows to be executed, as in the experimental **protocol**
- Research institution, country, and scientific domain of the RO
- The actual **size** of the RO and/or a folder
- The **version** of a workflow

Research Object Wf4Ever Semantic Model

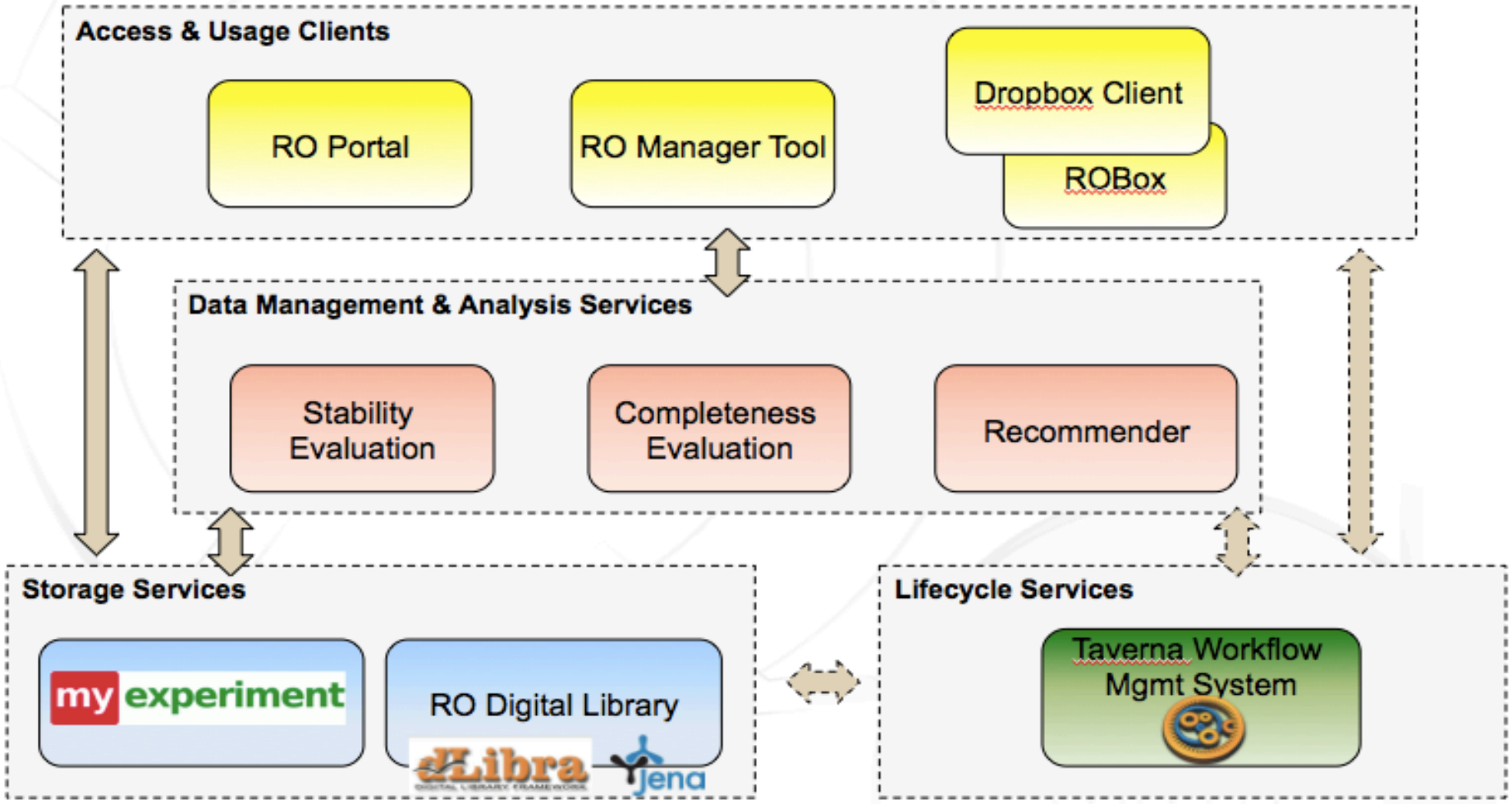


VOTable DataLink

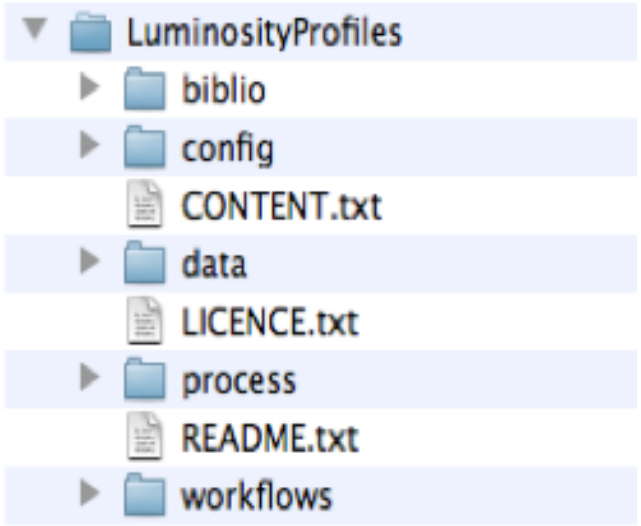
Research Object Digital Library Architecture



Research Object Digital Library Architecture



Luminosity Profiles RO



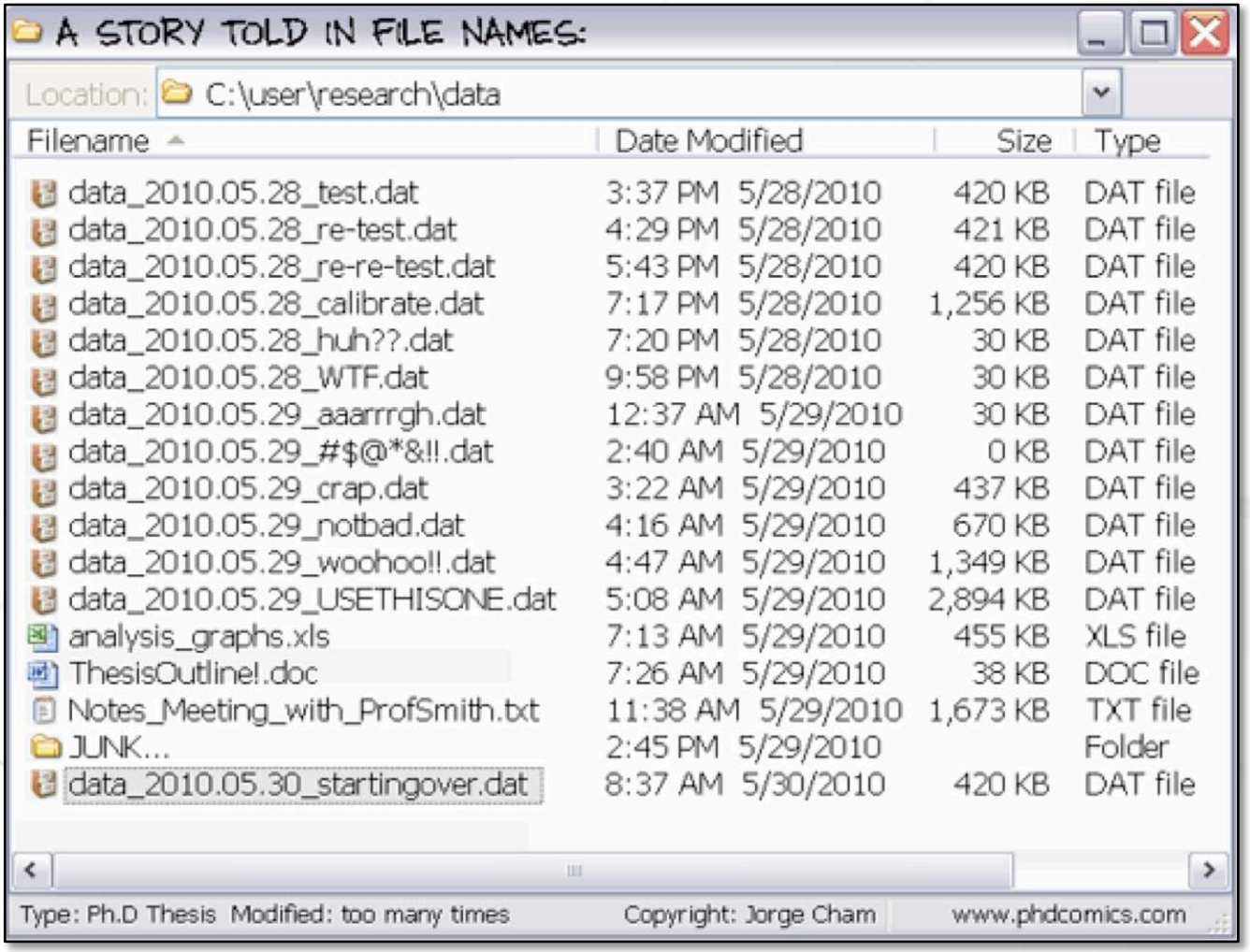
1010 Files, 200 MB
External Sources ~ 8 GB

5 Main Workflows, 14 Nested Workflows, 25 Scripts, 11 Configuration files
10 Software dependencies, 1 Web Service

Dataset: 90 galaxies observed in 3 bands

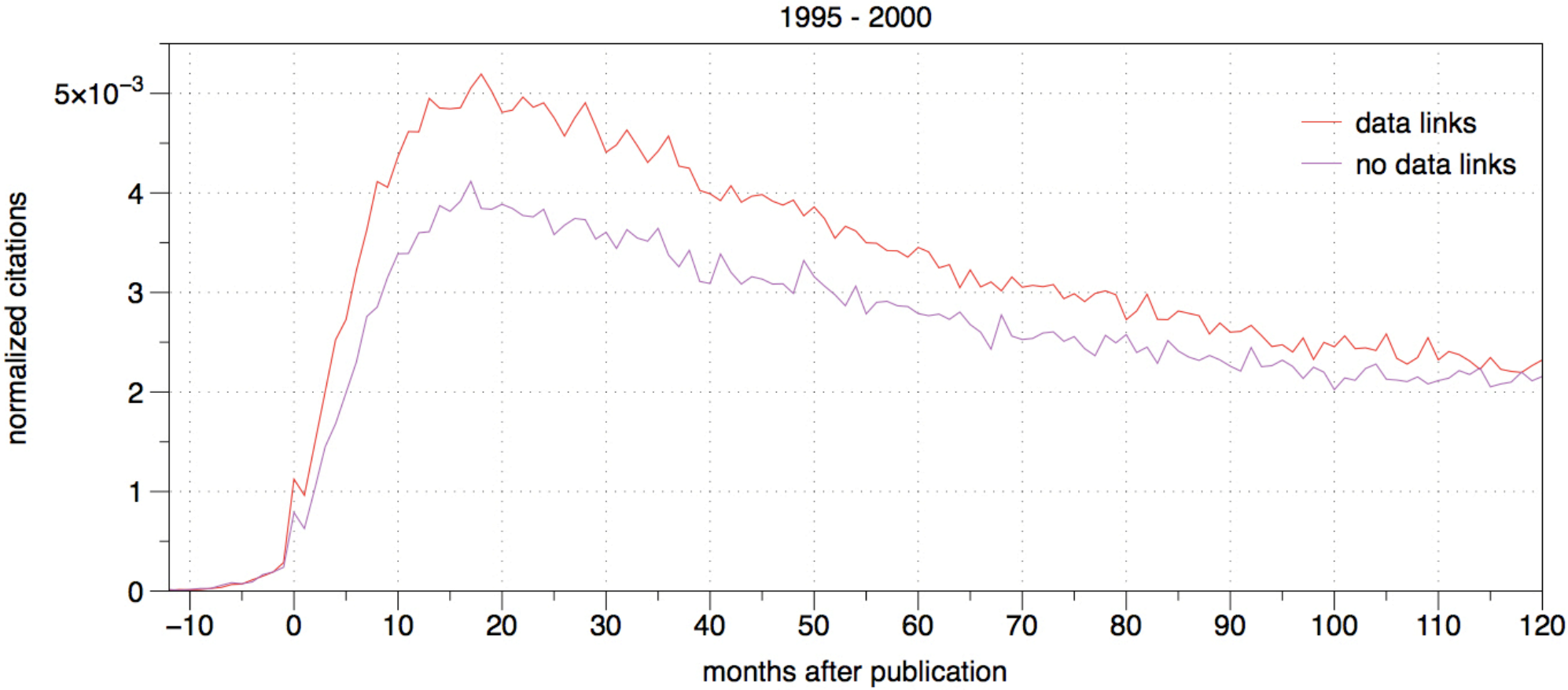
Reproducibility

When organization is better than automation



Credit and attribution

Papers with data links are cited more than those without

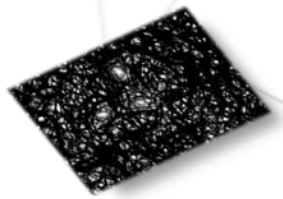


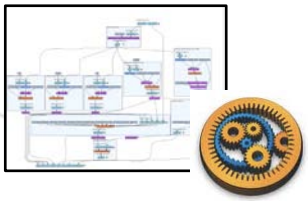
Effect of E-printing on Citation Rates in Astronomy and Physics
2006. Edwin A. Henneken et al.

ADSLabs Research Objects

ADO Linked Components

- Authors
- Publications
- Journals
- Objects SIMBAD
- Tabular data behind the plots CDS
- ASCL reference of used software
- Observing time Proposals
- Used facilities, surveys or missions





The next generation of archives

Much wider FoV and spectral coverage

- Huge sized datasets (~ tens TB)
- Big Data science highly dependent on I/O data rates
- Subproducts as virtual data generated on-the-fly

We are moving into a world where

- **computing and storage are cheap**
- **data movement is death**

The next generation of archives

Much wider FoV and spectral coverage

- Huge sized datasets (~ tens TB)
- Big Data science highly dependent on I/O data rates
- Subproducts as virtual data generated on-the-fly

The *move computing to data* paradigm

Archives should evolve from data providers into **services providers**, where web services may help to solve bandwidth issues.

The next generation of archives

Much wider FoV and spectral coverage

- Huge sized datasets (~ tens TB)
- Big Data science highly dependent on I/O data rates
- Subproducts as virtual data generated on-the-fly

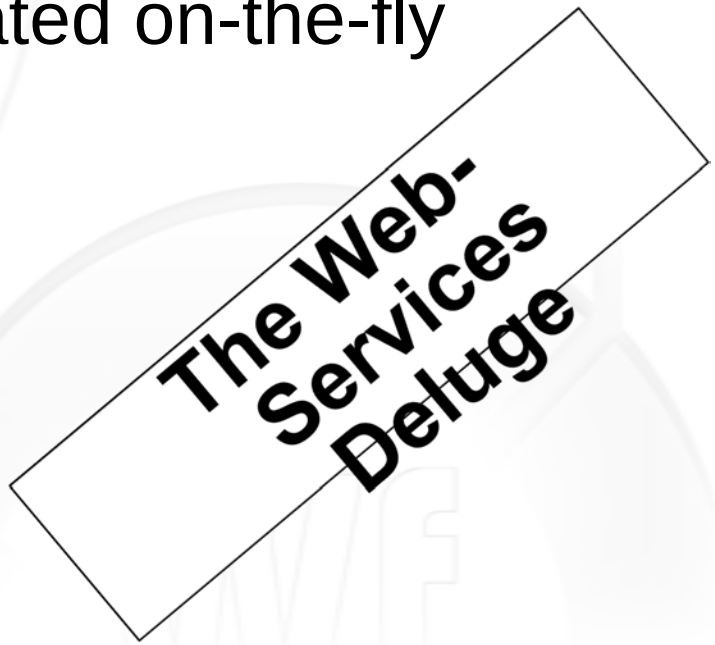
Data Discovery
Data Access
Data Management

The next generation of archives

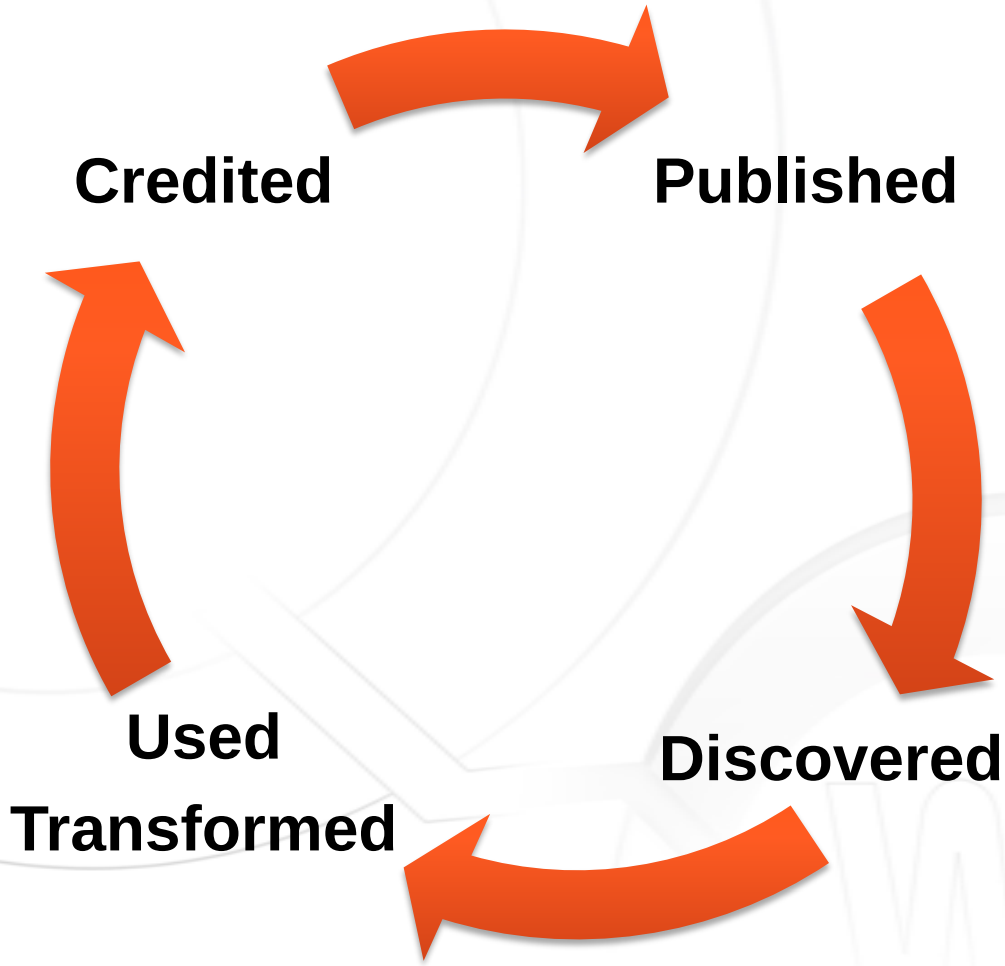
Much wider FoV and spectral coverage

- Huge sized datasets (~ tens TB)
- Big Data science highly dependent on I/O data rates
- Subproducts as virtual data generated on-the-fly

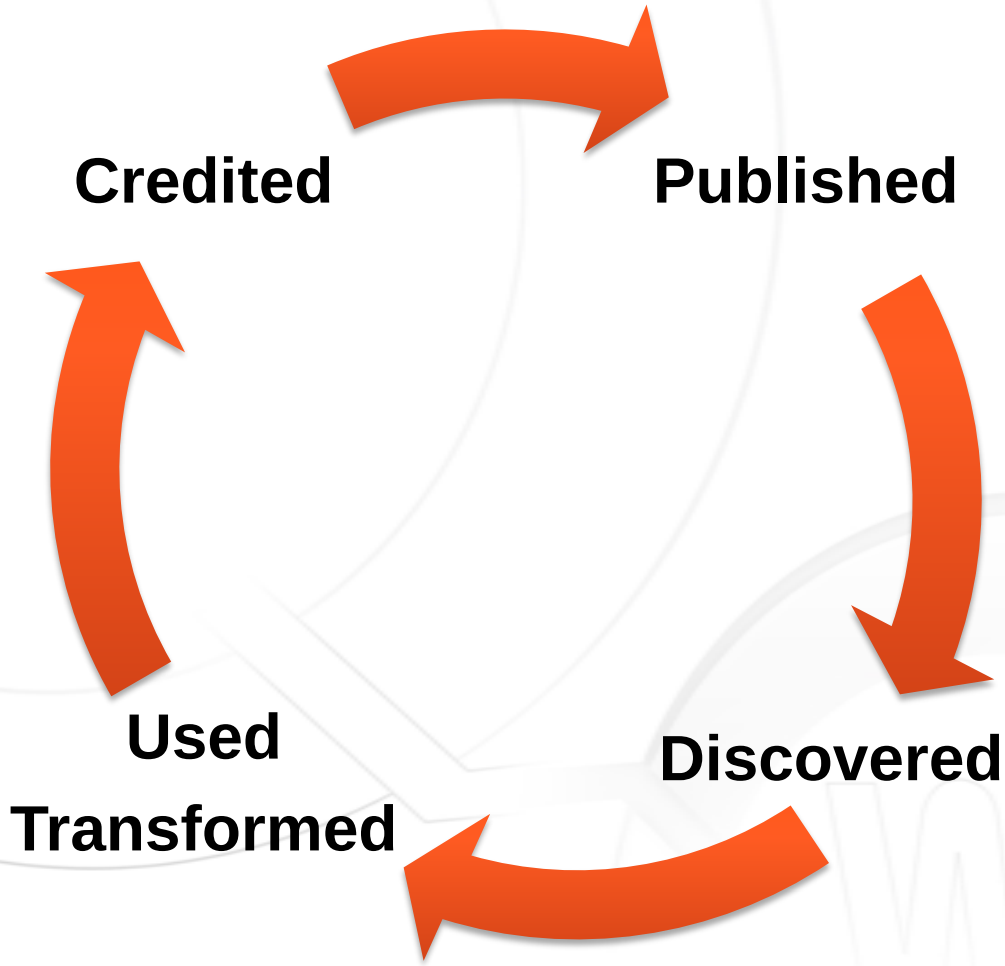
Web Services Discovery
Web Services Access
Web Services Management



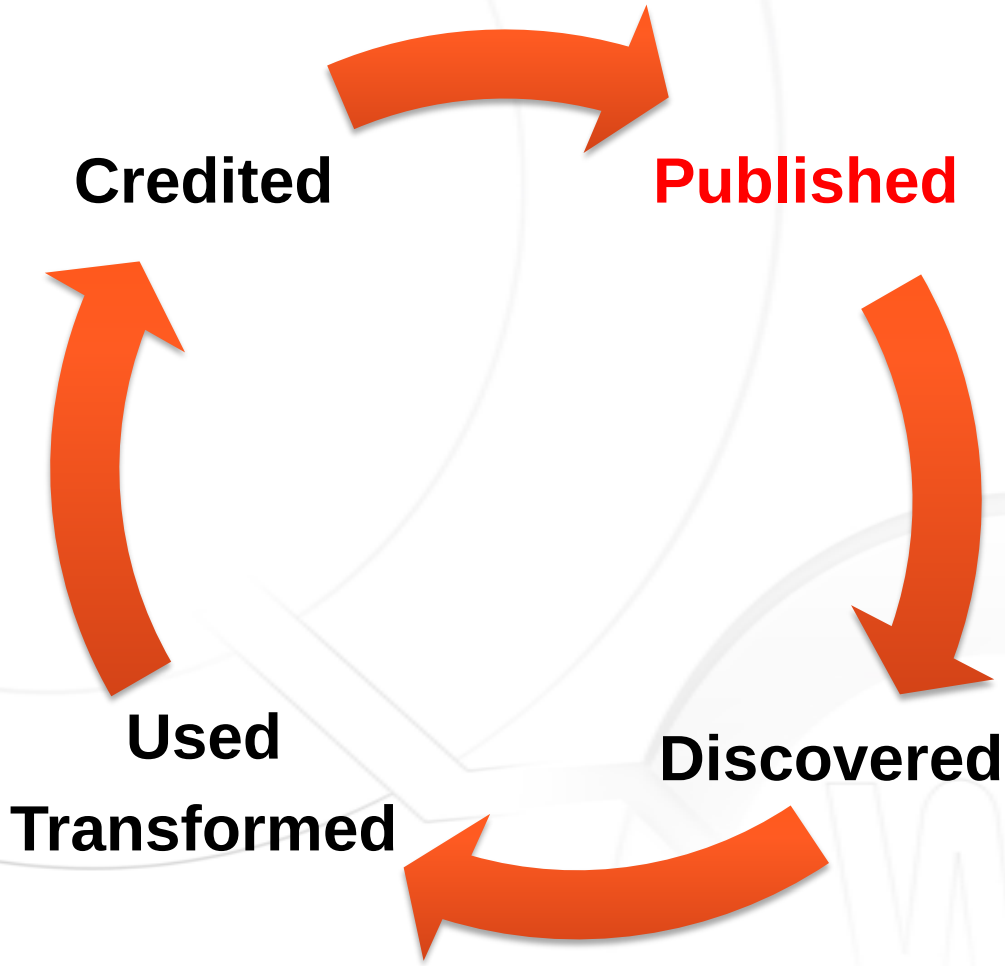
The Data Lifecycle



The Service Lifecycle



The Service Lifecycle

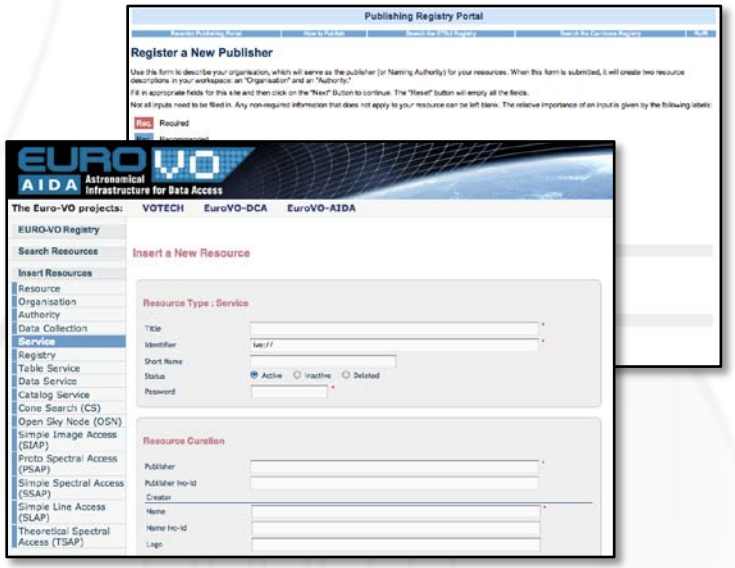


Published

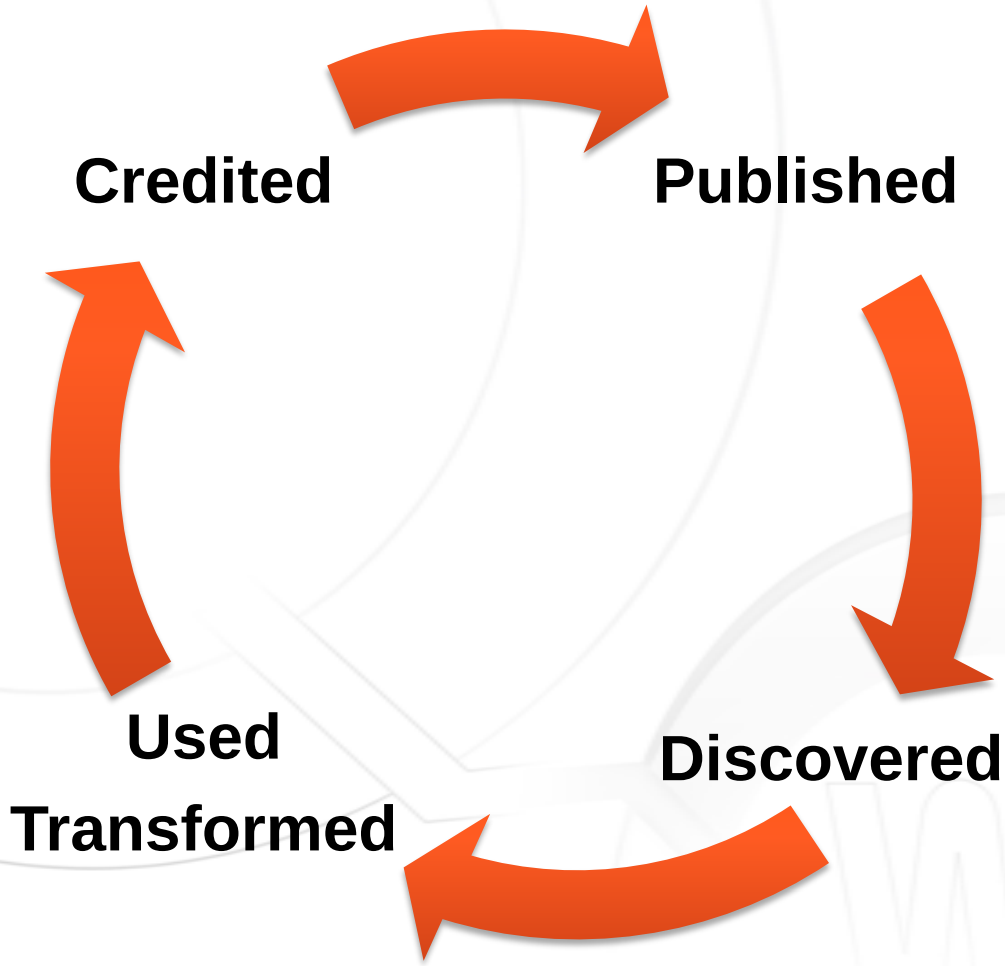
- The VO Registry
- Easier to publish services than datasets in the VO ?
- WS are not exclusive property of big data archives

- Publication is not Preservation
- Backup strategies
- Replication/Mirrors
- Versioning

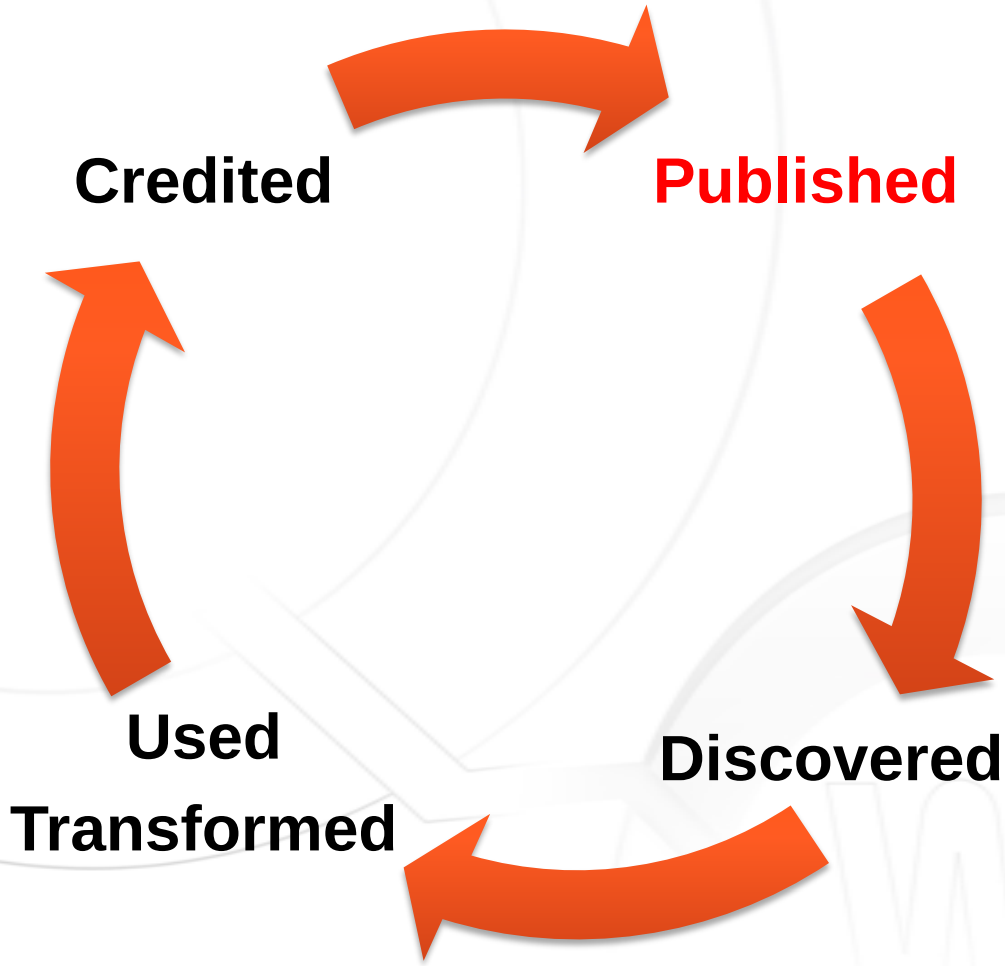
- Software Publishing Platforms



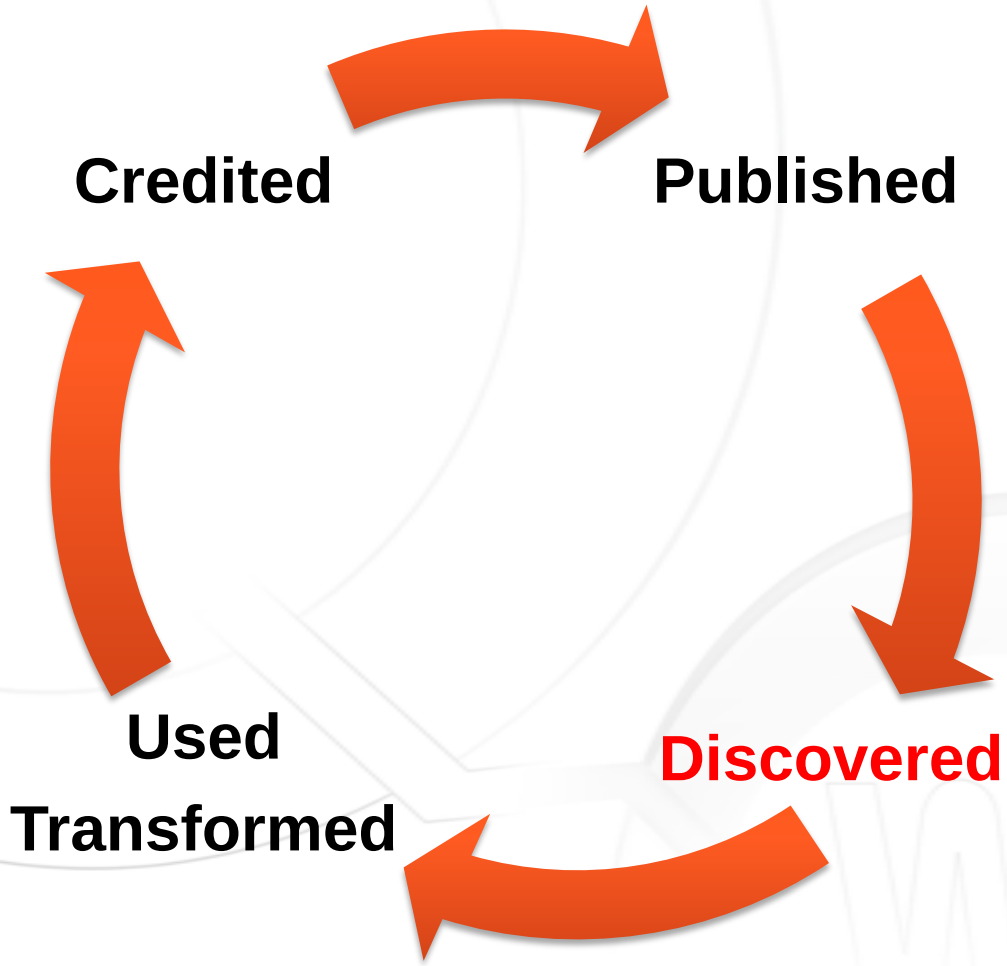
The Service Lifecycle



The Service Lifecycle



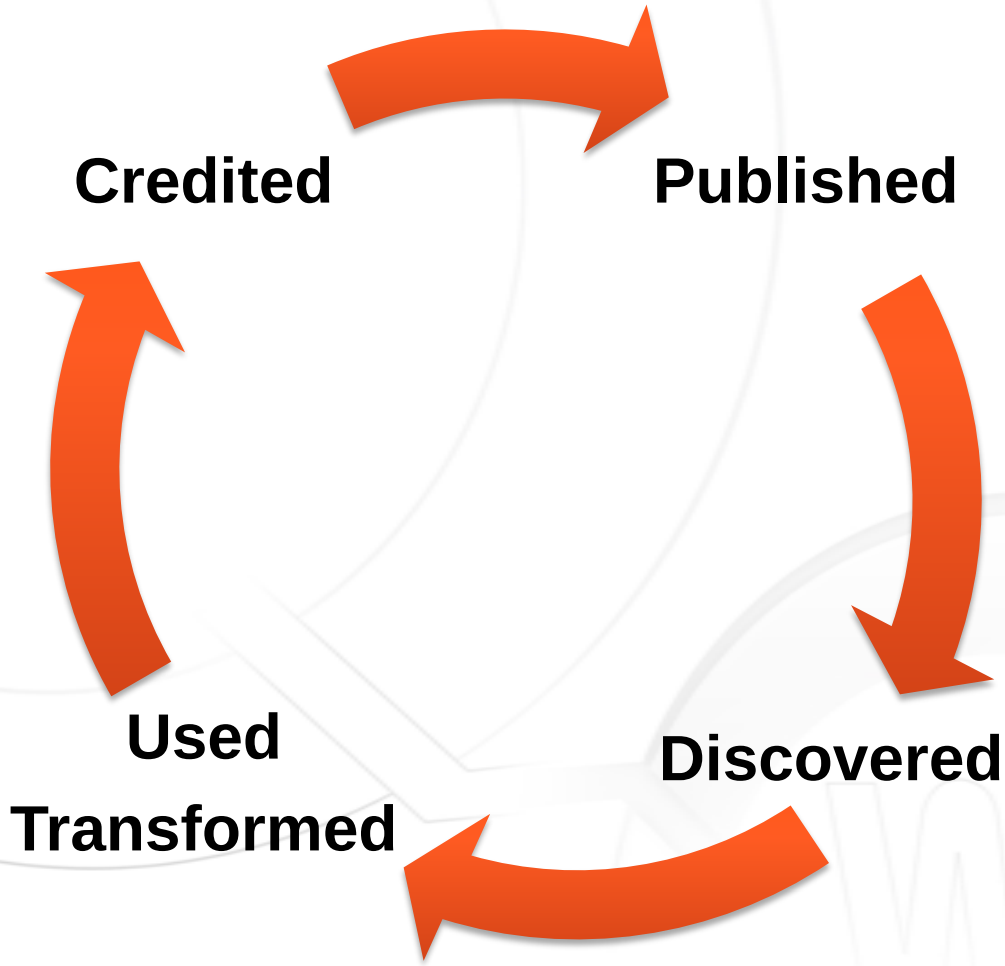
The Service Lifecycle



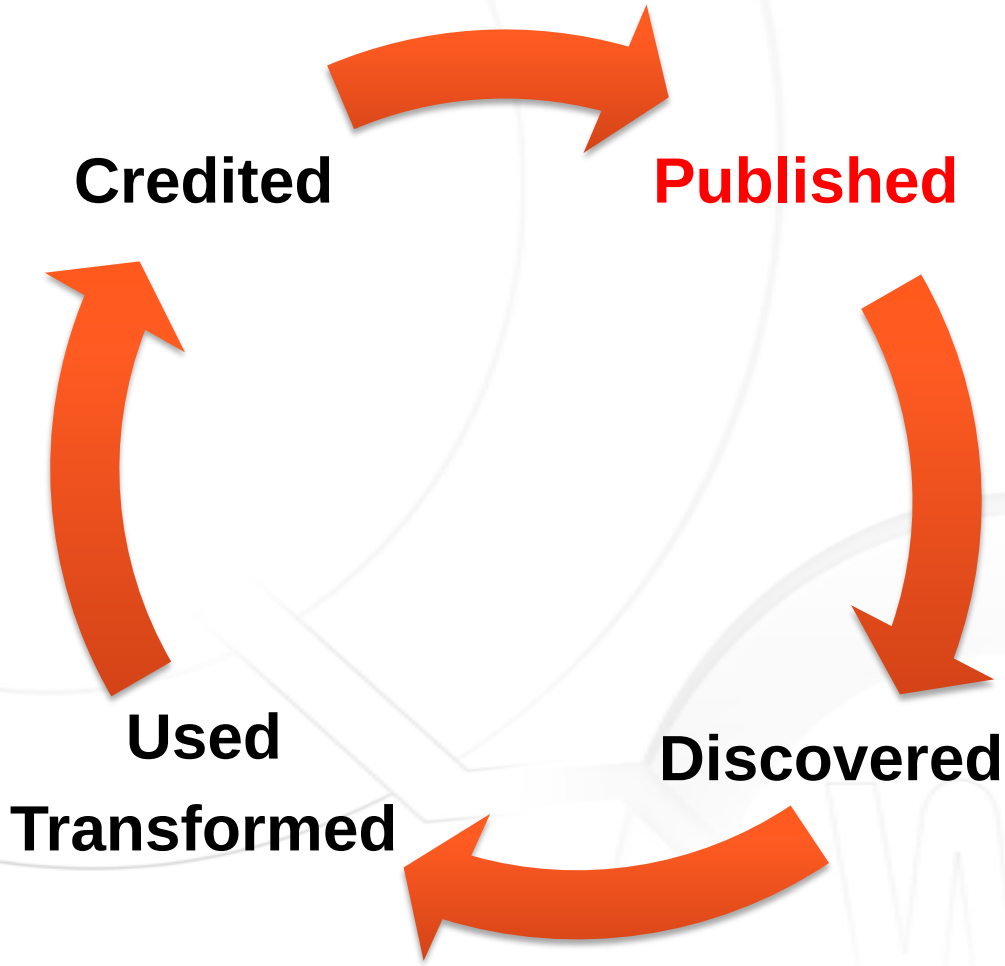
Discovered

- **Search Criteria**
  - Relevant Keywords (Semantics)
  - Authoring - Institution, Archive
  - Waveband, Science
  - Function-based
    - VO Services mainly focused on Data Discovery and Access (DAL)
    - Wrapped Legacy Apps and Data Processing (SIAv2, Theory IG)
    - KDD IG
  - Input/Output Data (TAP, UTypes, VOSI #tables)
  - Access Policy (Authentication – SSO, OAuth)
  - A-Synchrony (SOAP, REST) and Stage Data (VOSpace)
  - Allocation of CPU/Storage, Estimated Computing Time
- **Proposition of alternatives and similars**

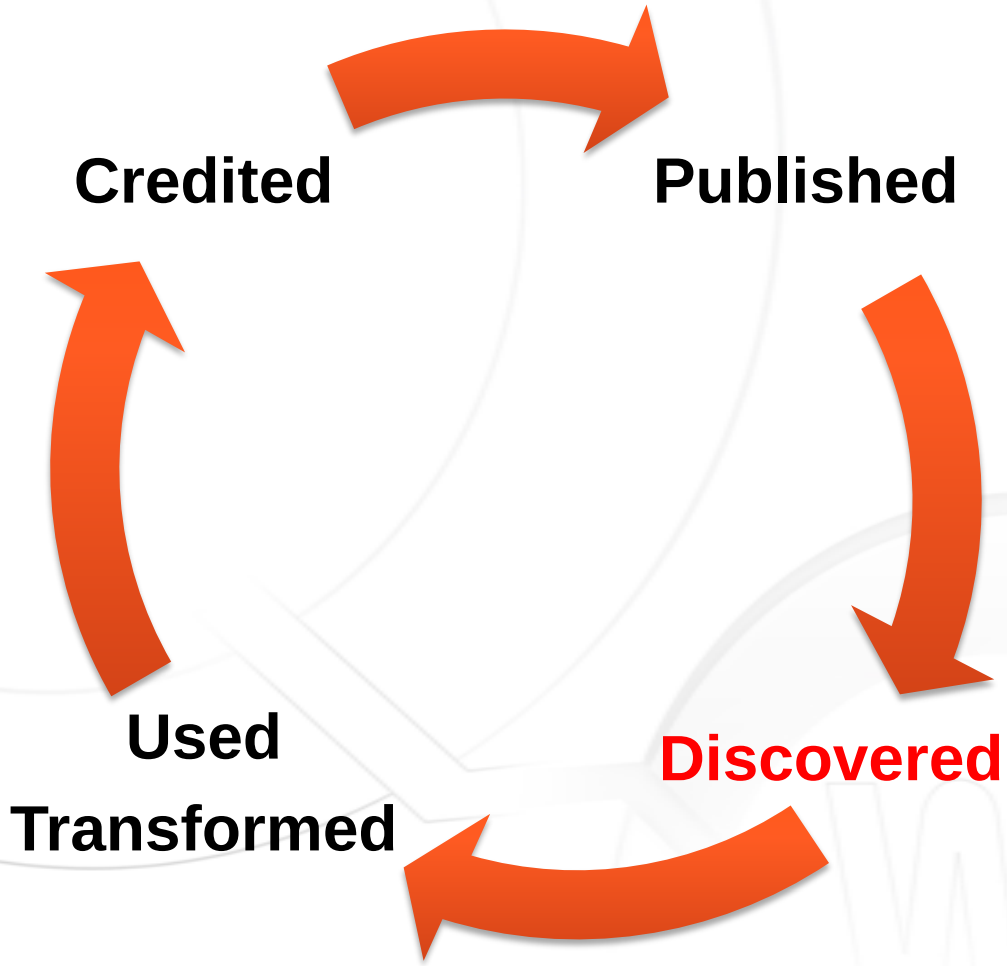
The Service Lifecycle



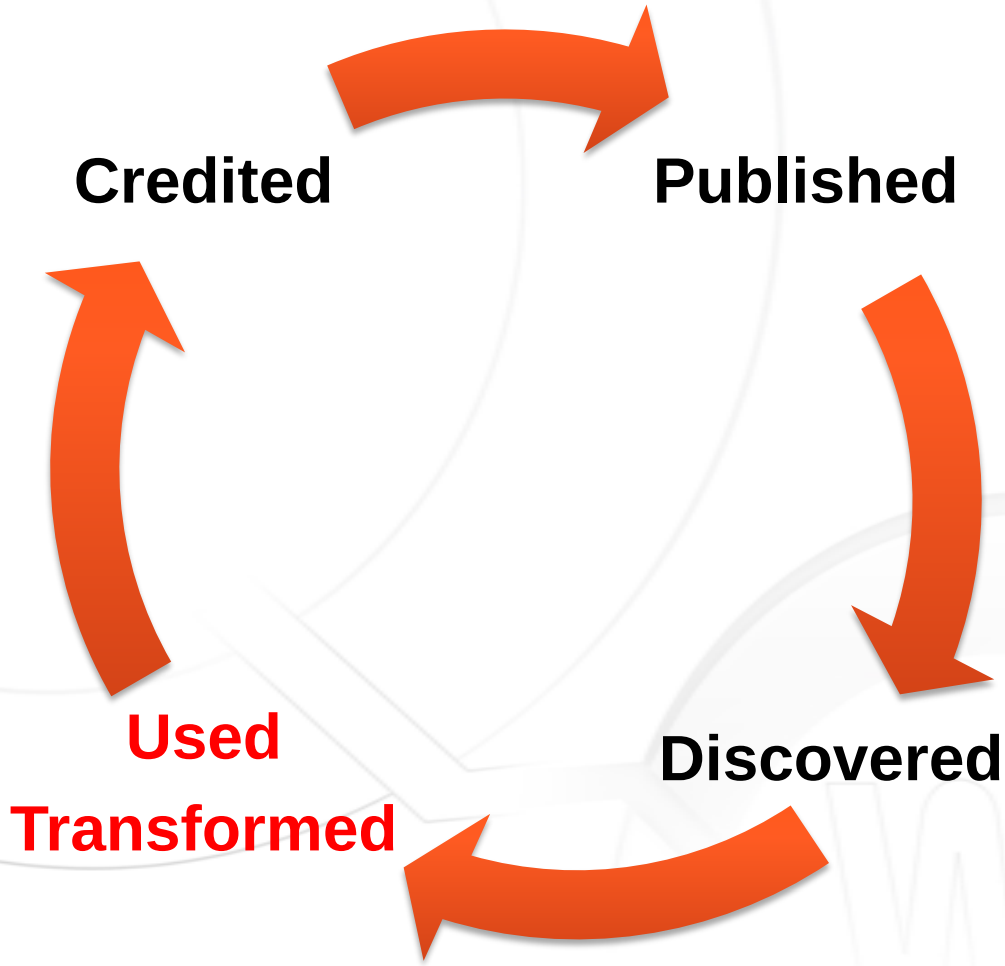
The Service Lifecycle



The Service Lifecycle

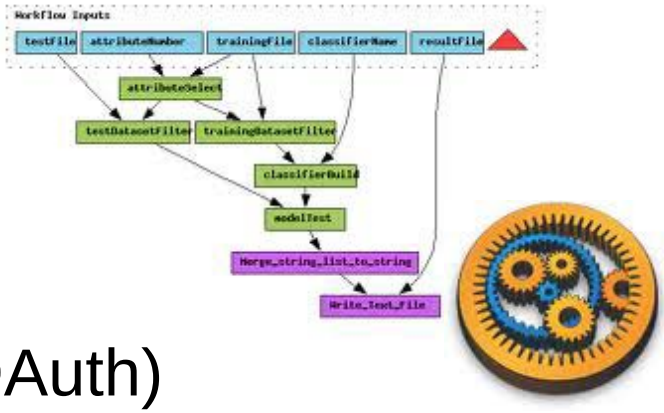


The Service Lifecycle



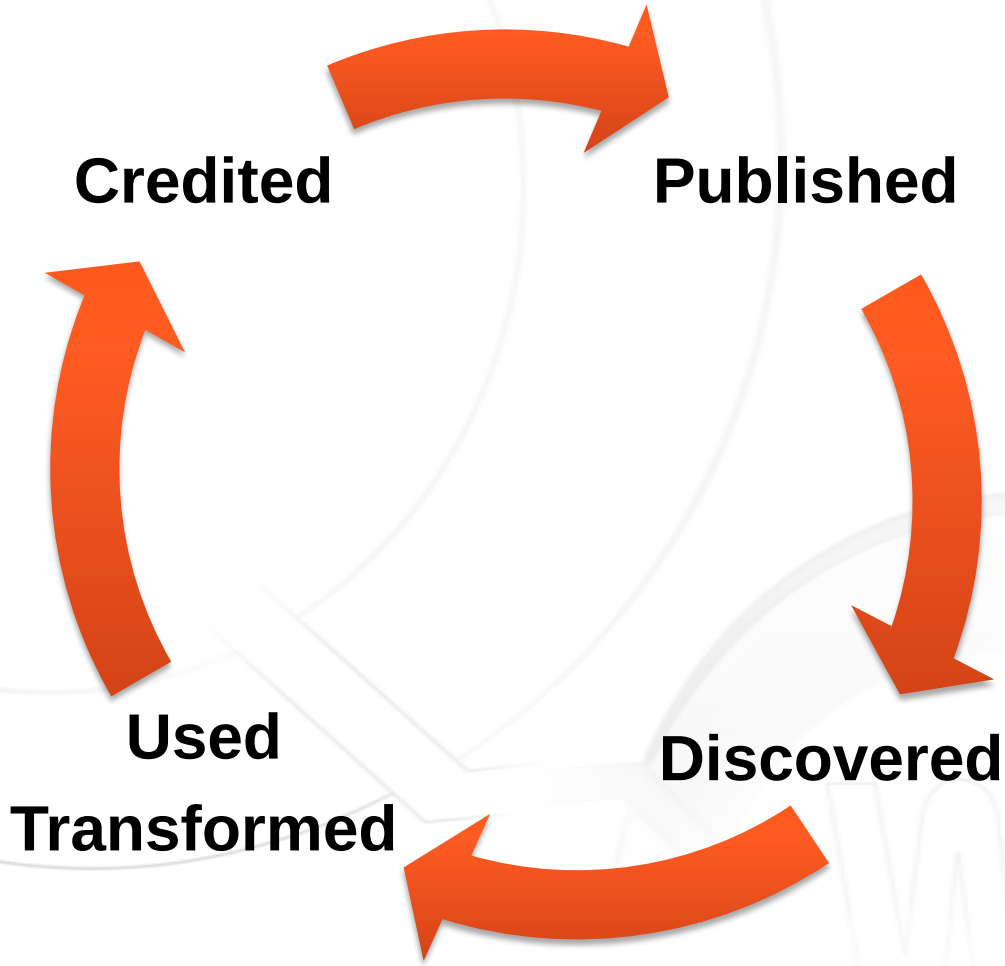
Used and Transformed

- **How to use them ?** (WADL, WSDL – VOSI #capabilities)
  - Input Data -> Parameters needed and formats
  - Self-described WS (PDL, S3, SimDAL, SimDB)
  - Output Data -> Response format - TAP
  - Example Data, Self-Consistency Checking

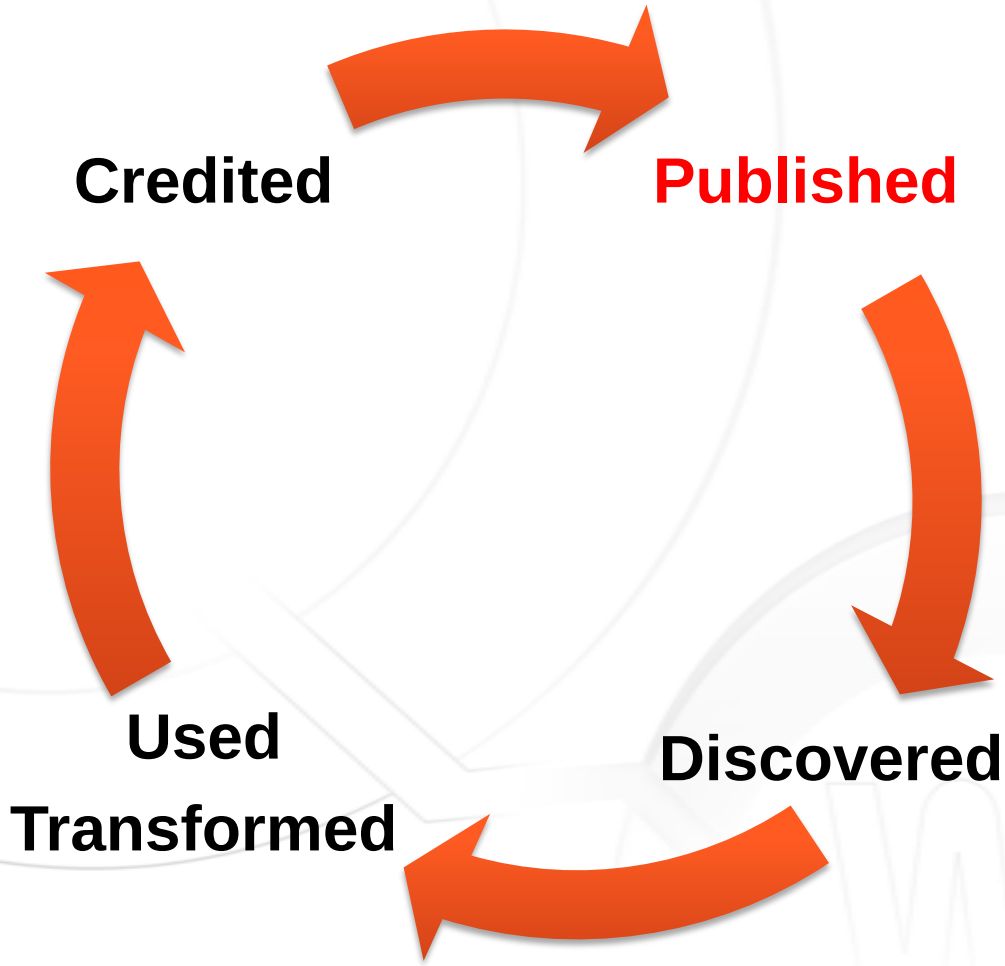


- Access Policy (**Authentication** – SSO, OAuth)
- **WS orchestration in Workflows** (Data-flow vs. Control-flow)
- How the **community** uses WS ?
- Propositions based on patterns of statistical use or popularity
- **Provenance** of the methods is Wf-evolution by re-use
- Consumed by Humans and Machines - **Interoperable** (WS-I)

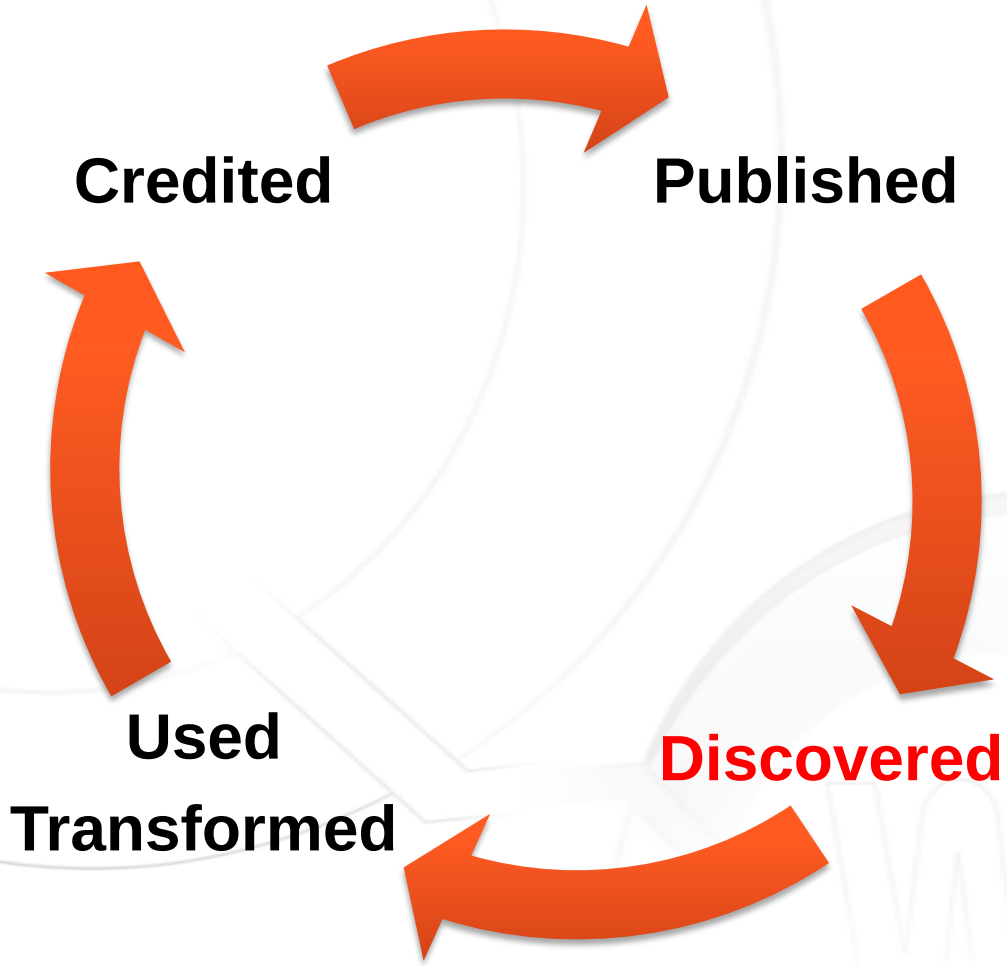
The Service Lifecycle



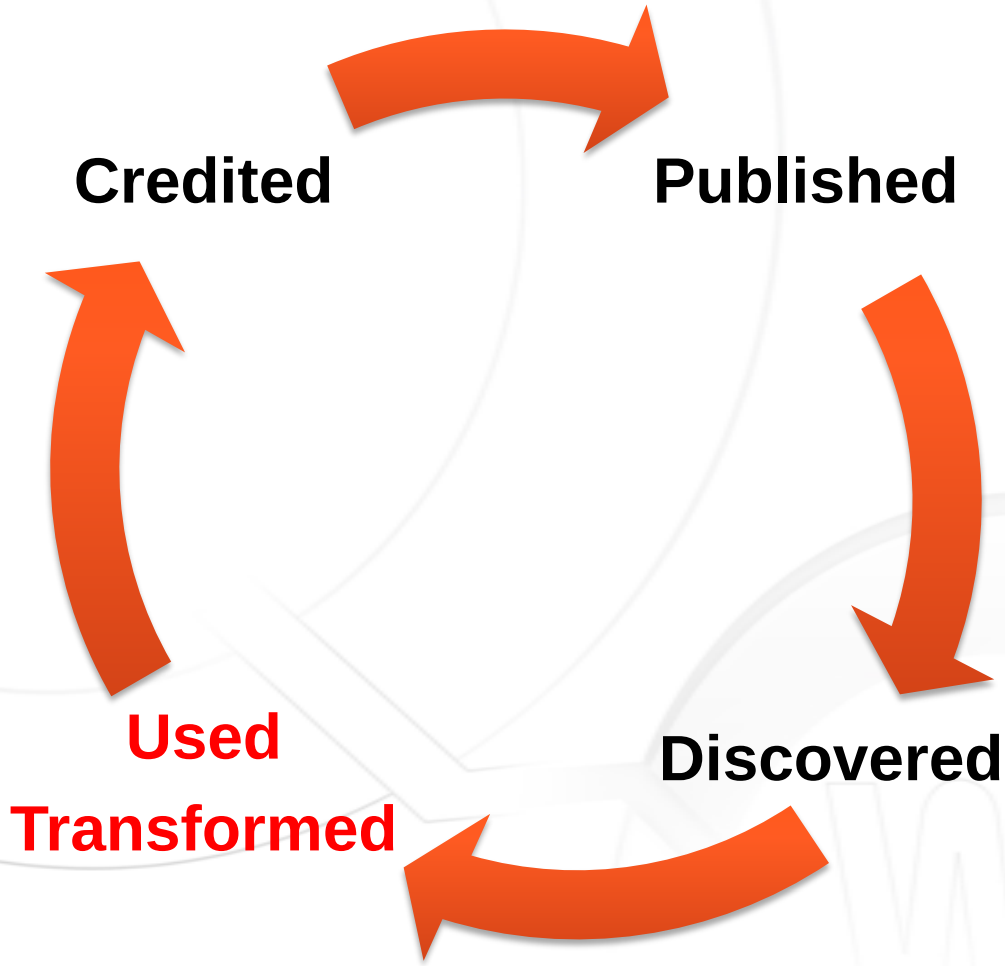
The Service Lifecycle



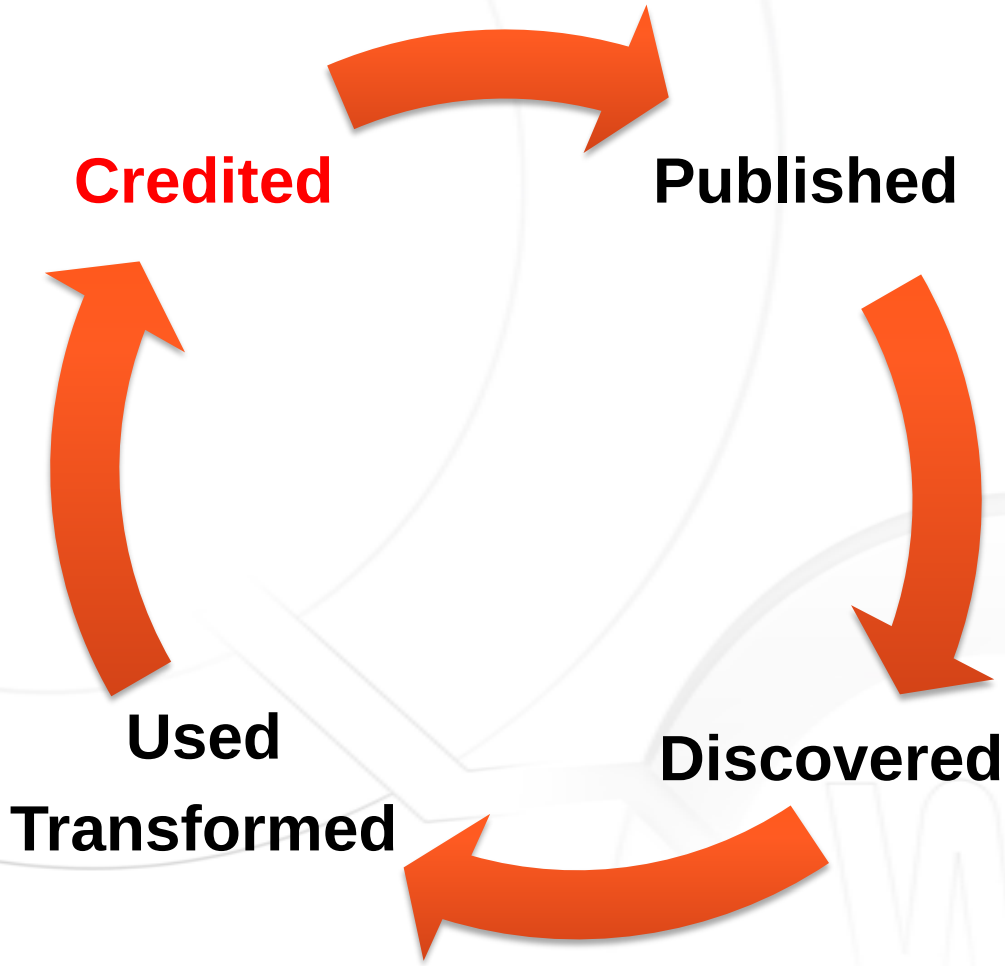
The Service Lifecycle



The Service Lifecycle

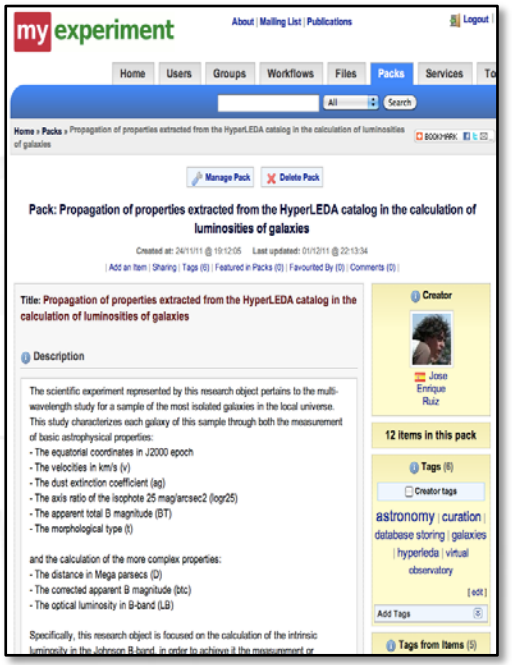


The Service Lifecycle



Credited

- **Linked to related Artefacts**
  - Data Facilities and Archives
  - Authors, ASCL Software, Wfs
- **Quality Assessment**
  - Technical and scientific
  - Penalize abandoned and award the maintained
- **Automate Monitoring (VOSI #availability)**
  - Decay
  - Performance, WS Analytics
  - Modifs. on interfaces, permissions, etc.
- **Community Curation**
  - Blogging
  - Recommendation
  - Folksonomy



In a cloud of web services and data..

Web Services should benefit of the *same privileges* acquired by Data until now.

Start thinking on how to provide

- **Detailed curation**
- **Thorough characterization**