



From Scientific Workflows to Research Objects: Publication and Abstraction of Scientific Experiments

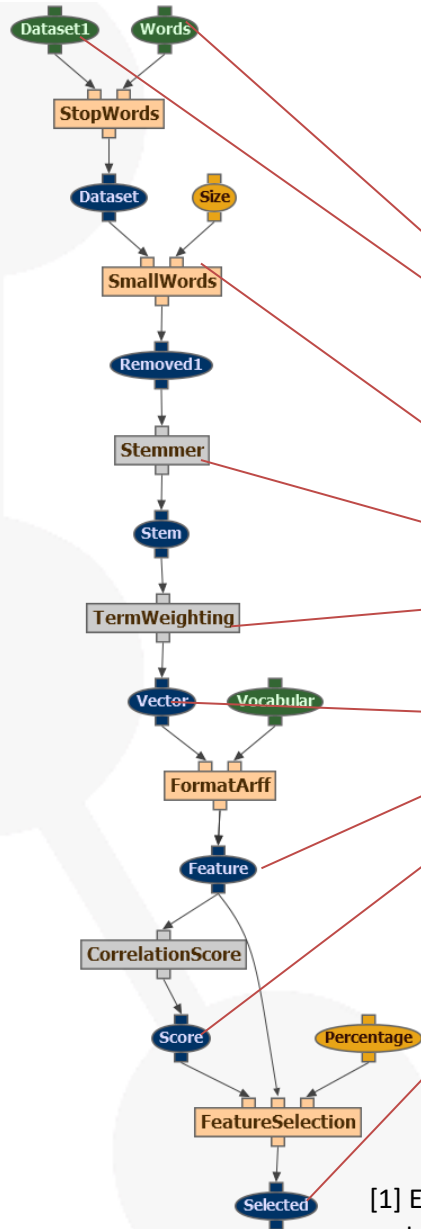
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Facultad de Informática
Universidad Politécnica de Madrid

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 - Linked Data
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6. Common motifs among scientific workflows
 - Workflow motif catalog
7. Detecting common fragments among scientific workflows
8. Workflows as part of an experiment: Research Objects



• “Template defining the set of tasks needed to carry out a computational experiment” [1]

• Inputs

• Steps

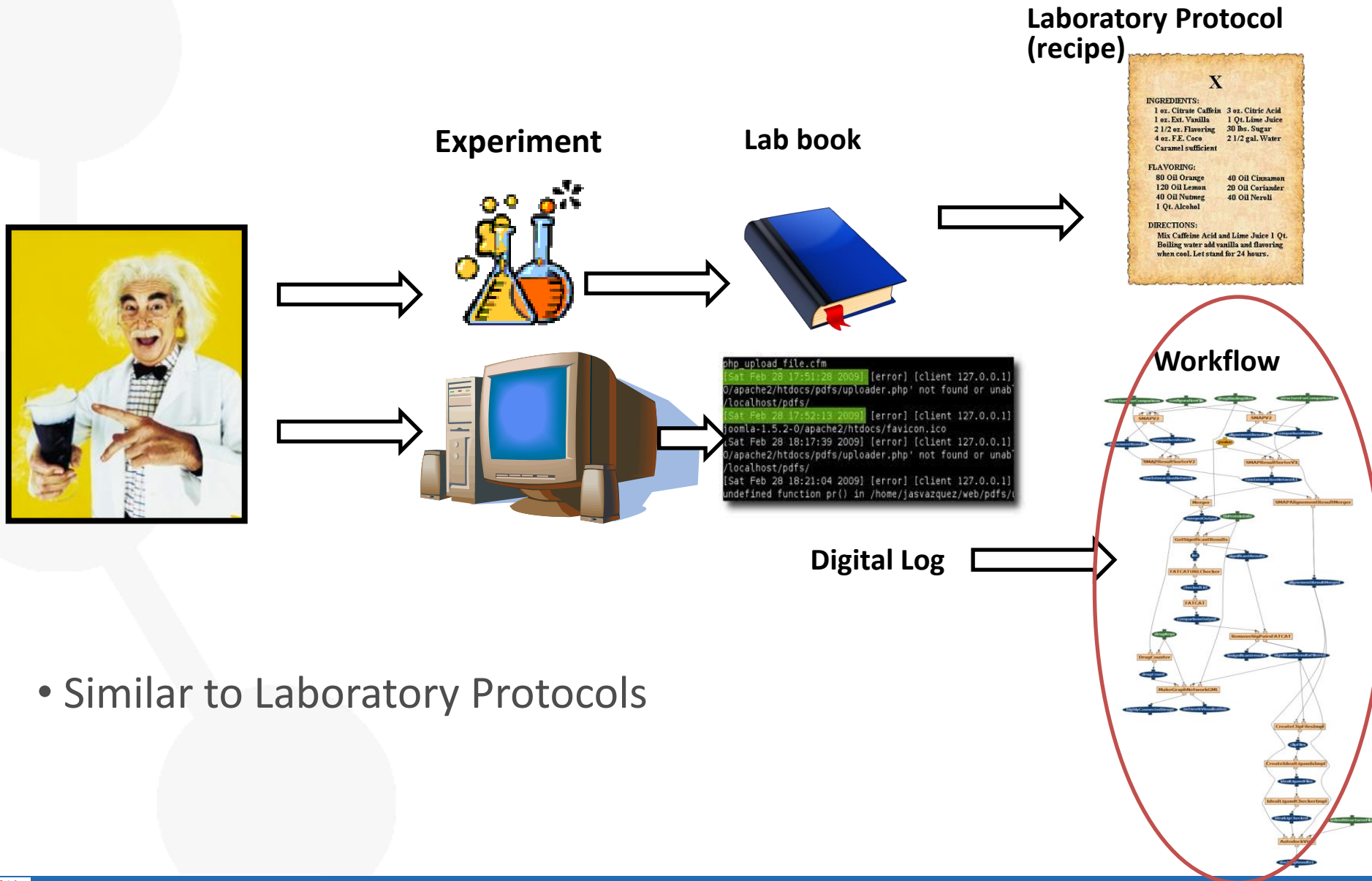
• Intermediate results

• Outputs

• Data driven, usually represented as **Directed Acyclic Graphs (DAGs)**

[1] Ewa Deelman, Dennis Gannon, Matthew Shields, Ian Taylor, Workflows and e-science: an overview of workflow system features and capabilities, Future Generation Computer Systems 25 (5) (2009) 528–540.

How are scientific workflows created?



- Workflow **representation**

- Plan/template representation
- Provenance trace representation
- Link between templates and traces

CH1: Can we export an abstract template of the method being represented?

CH2: How do we interoperate with other workflow results?

CH3: How do we access the workflow results?

CH4: How do we link an abstract method with several implementations?

- Creation of **abstractions/motifs** in scientific workflows

- Abstraction **catalog**
- Find how different workflows are related

CH5: How can we detect what are the typical operations in scientific workflows?

CH6: How can we detect them automatically?

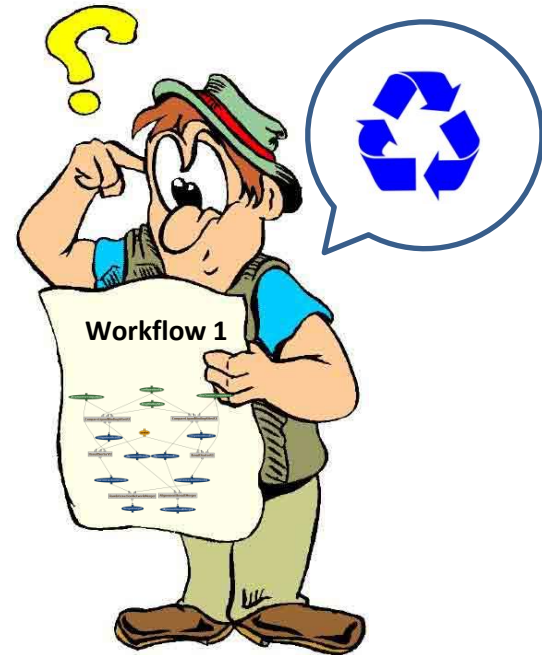
- Understandability and reuse** of scientific workflows

- Relation between the workflows involved in the same experiment
(**Research Objects**)

CH7: Which workflow parts are related to other workflows?

CH8: How do workflows depend on the other parts of the experiments?

- As a **designer: Discovery**
 - Workflows with similar functionality fragments/methods
 - Design based in previous templates.
- As **user/reuser: Understandability, Exploration**
 - Search workflows by functionality
 - Commonalities between execution runs
 - Component categorization



Abstraction definitions and categorization

Descriptions/
PSMs/Ontologies

Algorithms for finding the different
abstractions automatically

Data mining tools,
graph analysis, etc.

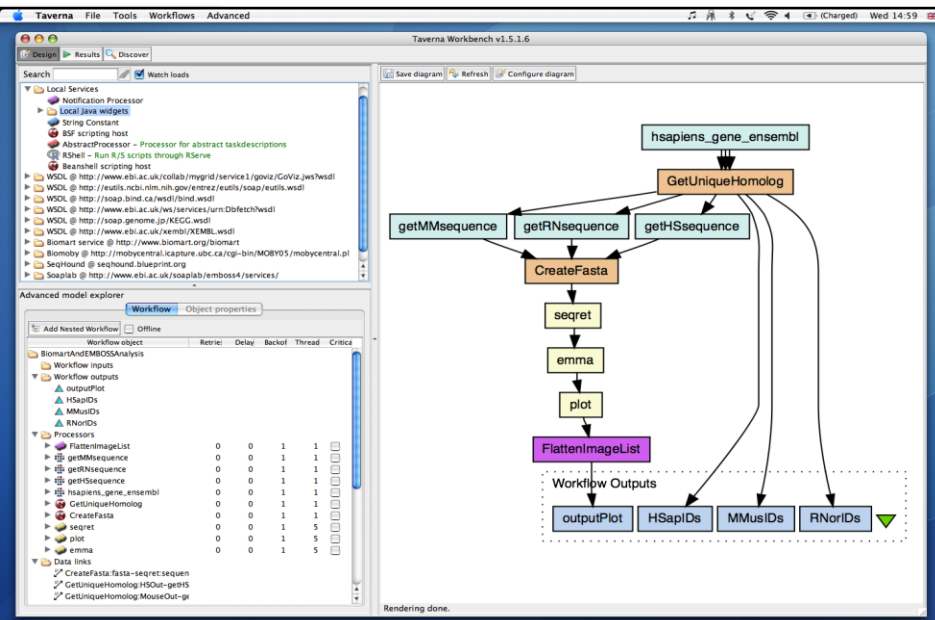
Experiment publication

RDF Stores

Provenance
representation

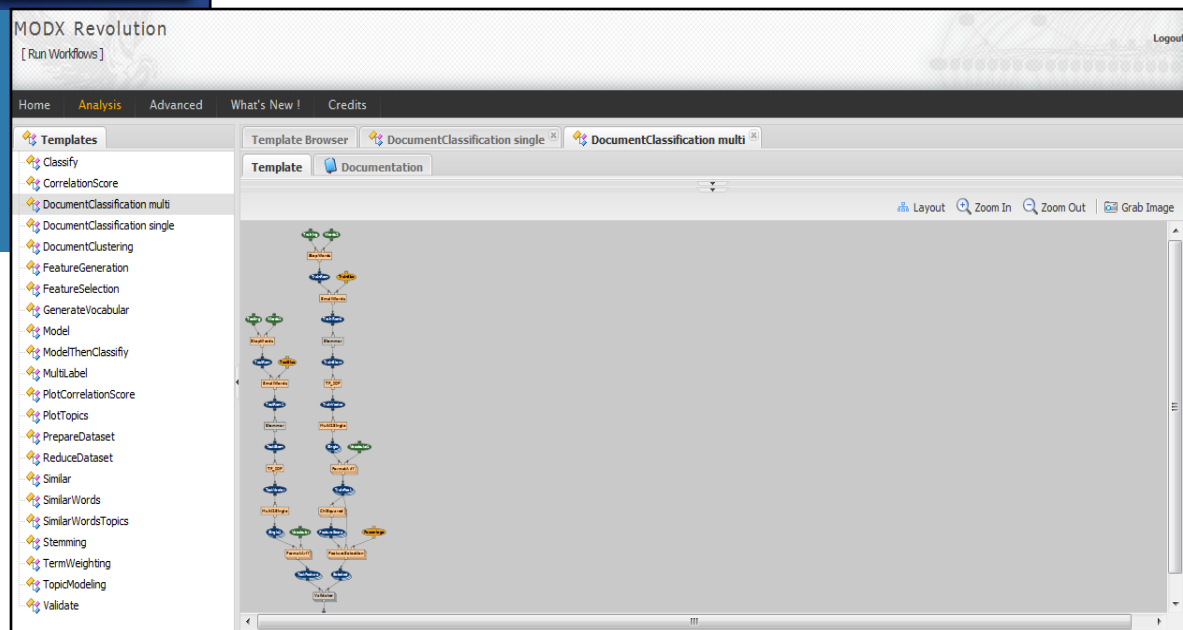
Plan
representation

Vocabularies



Taverna

<http://www.taverna.org.uk/>



<http://www.wings-workflows.org/>

Representing and publishing scientific workflows in the Web



A New Approach for Publishing Workflows: Abstractions, Standards, and Linked Data. Garijo, D.; and Gil, Y. In *Proceedings of the 6th workshop on Workflows in support of large-scale science*, page 47-56, Seattle, 2011. ACM

Abstractions definitions and categorization

Algorithms for finding the different
abstractions automatically

Experiment Publication

Provenance
representation

Plan
representation

Virtuoso,
Pubby,
Wings (+Plugin)

OPMW

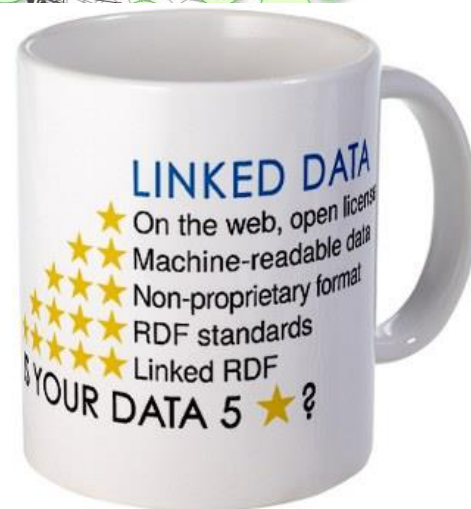
What is Linked Data?

1. Use URIs as names for things.

2. Use HTTP URIs so that people can look up those names.

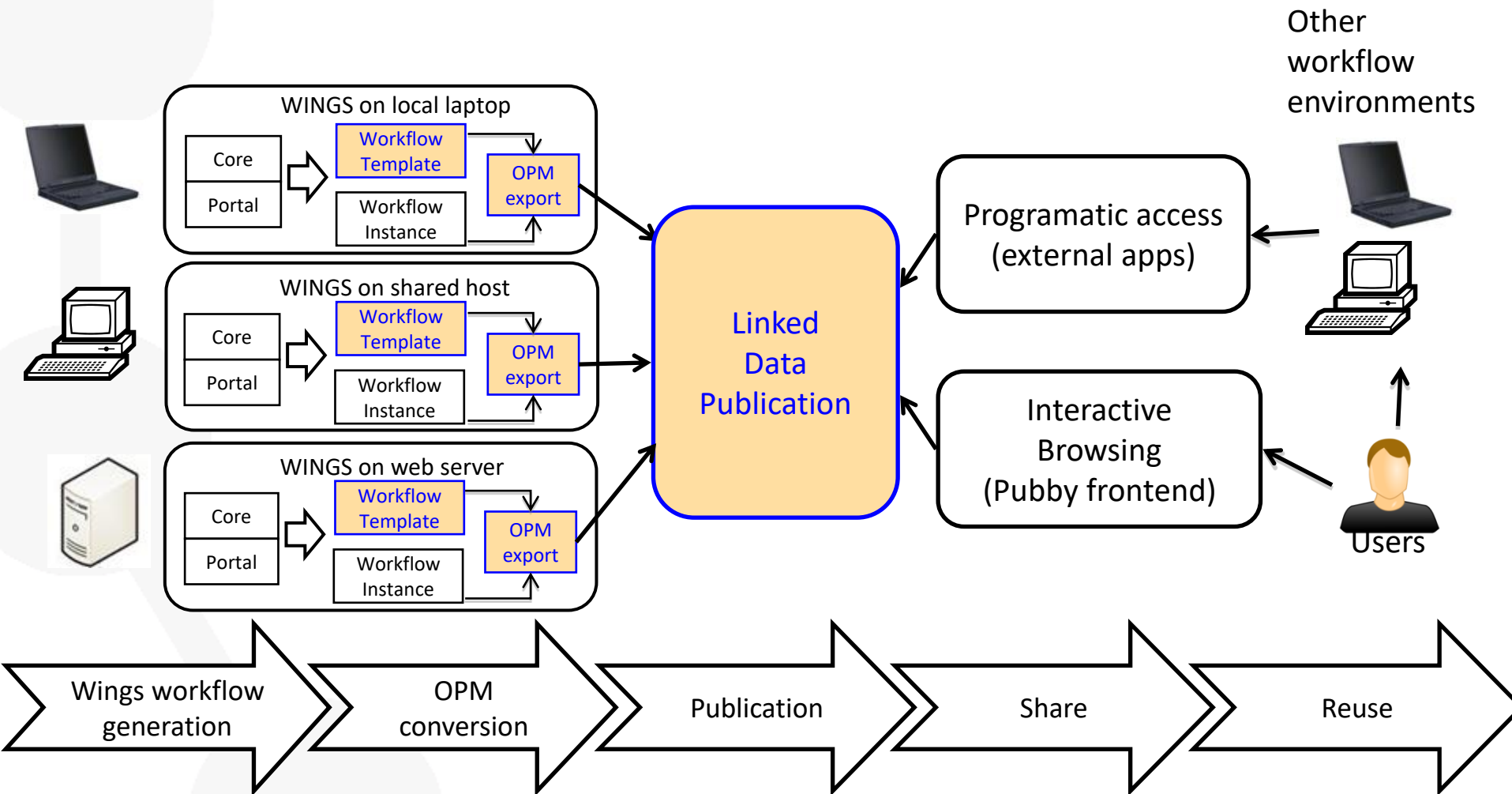
3. When someone looks up a URI, provide useful information.

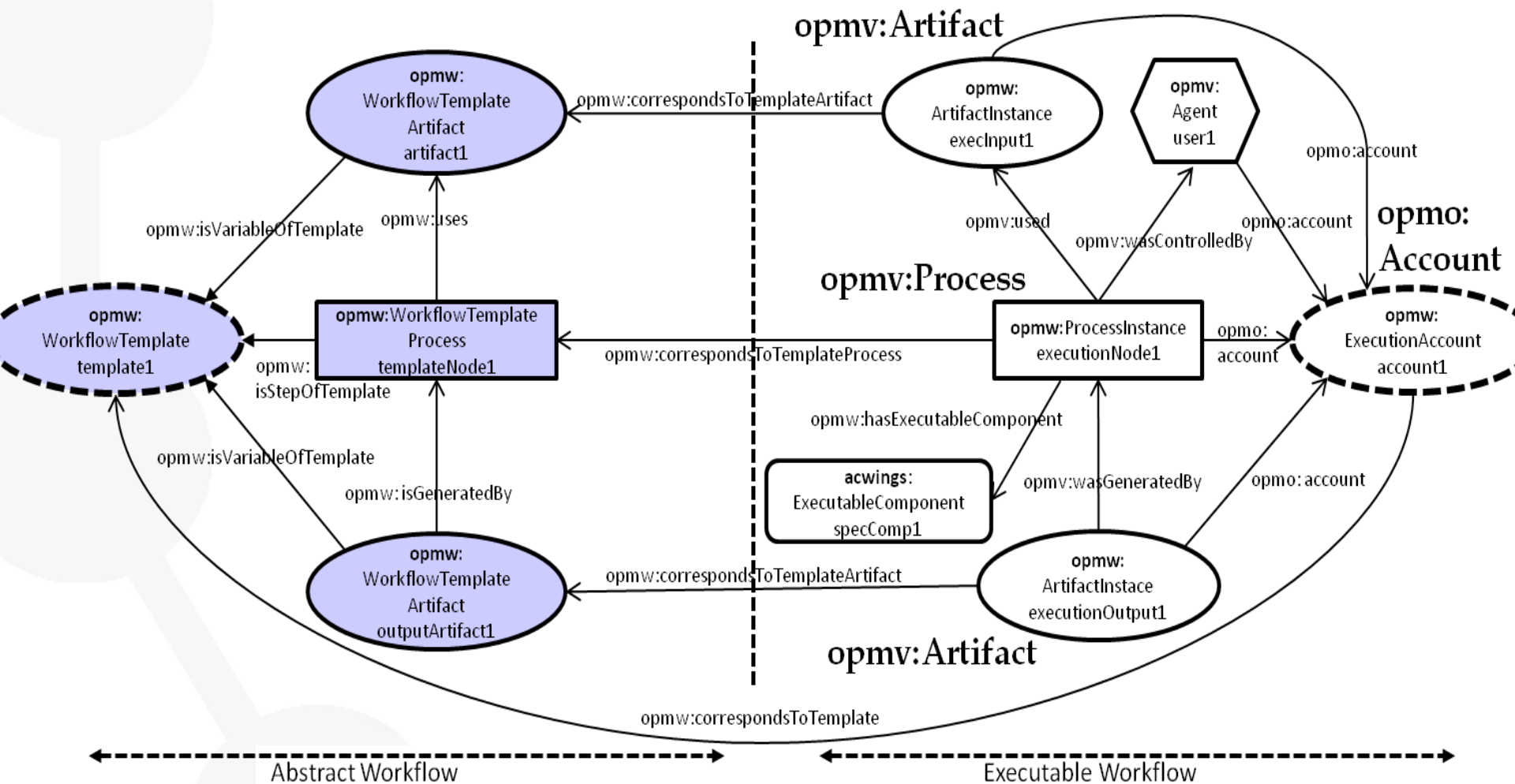
4. Include links to other URIs.



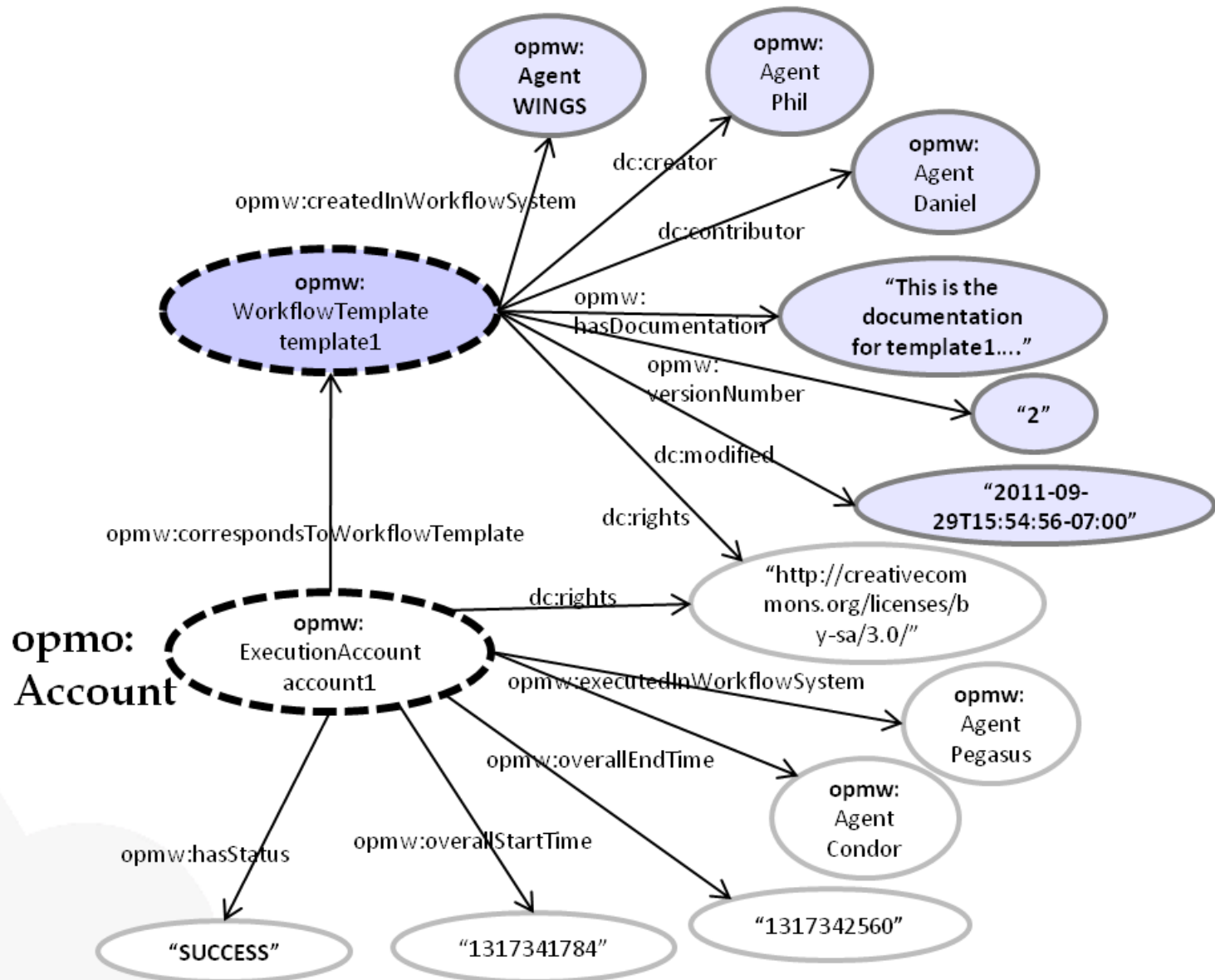
"Linking Open Data cloud diagram, by Richard Cyganiak and Anja Jentzsch. <http://lod-cloud.net/>"

Publishing workflows: high level architecture





<http://www.opmw.org/ontology/>



Standards



PROV-O: The PROV Ontology. Lebo, T.; Sahoo, S.; McGuinness, D.; Belhajjame, K.; Corsar, D.; Cheney, J.; Garijo, D.; Soiland-Reyes, S.; Zednik, S.; and Zhao, J. W3C Consortium. 2012.

Abstractions definitions and categorization

Algorithms for finding the different
abstractions automatically

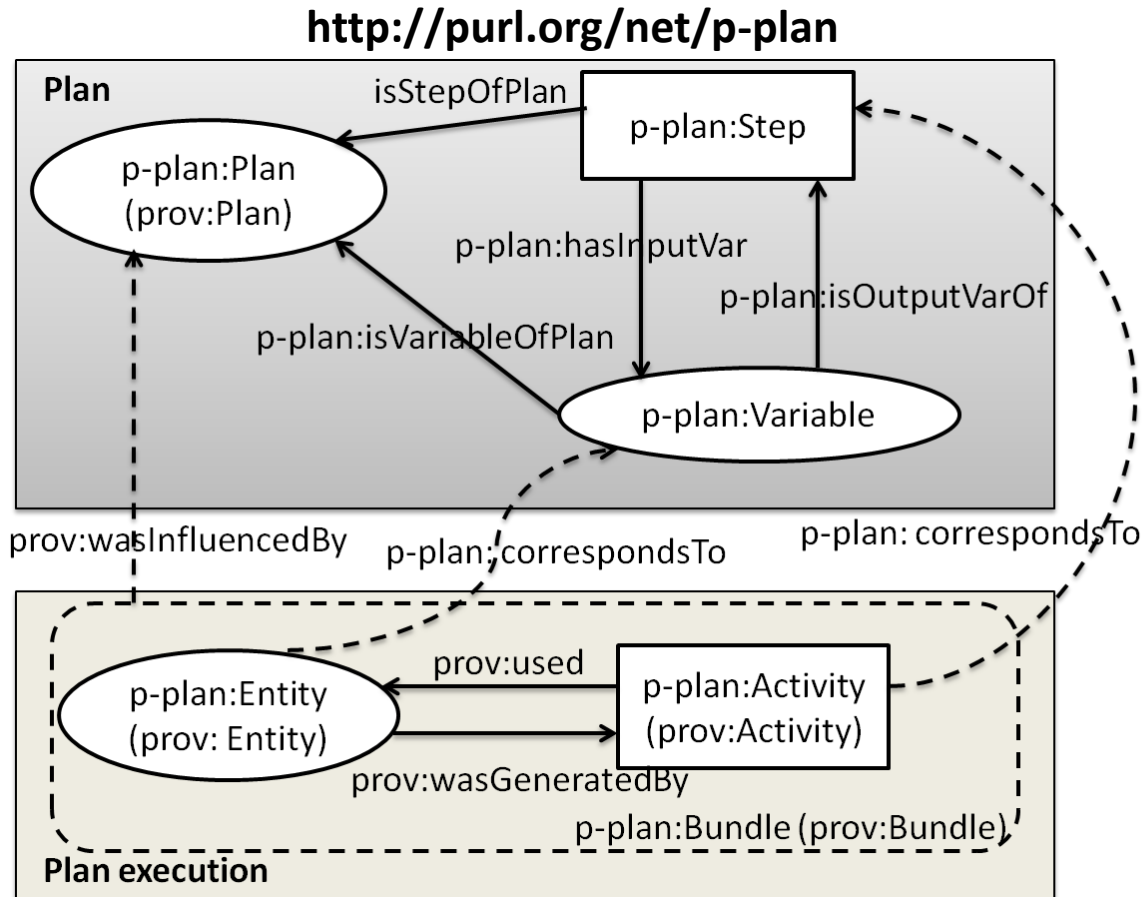
Experiment Publication

Virtuoso,
Pubby,
Wings (+Plugin)

Provenance
representation

Plan
representation

OPMW + PROV
+ P-PLAN



- Plans are **not provenance**
- **P-PLAN**: Simple plan model for binding traces to template representations
- Aligned with **OPMW and PROV (W3C Provenance Standard)**



Augmenting PROV with Plans in P-PLAN: Scientific Processes as Linked Data. Garijo, D.; and Gil, Y. In *Proceedings of the 2nd International Workshop on Linked Science 2012*, Boston, 2012.

Common motifs among scientific workflows



Common motifs in scientific workflows: An empirical analysis. Garijo, D.; Alper, P.; Belhajjame, K.; Corcho, O.; Gil, Y.; and Goble, C. *Future Generation Computer Systems*, . 2013

Abstractions definitions and categorization

Motif Detection

Algorithms for automatic matching

Experiment Publication

Virtuoso,
Pubby,
Wings (+Plugin)

Provenance
representation

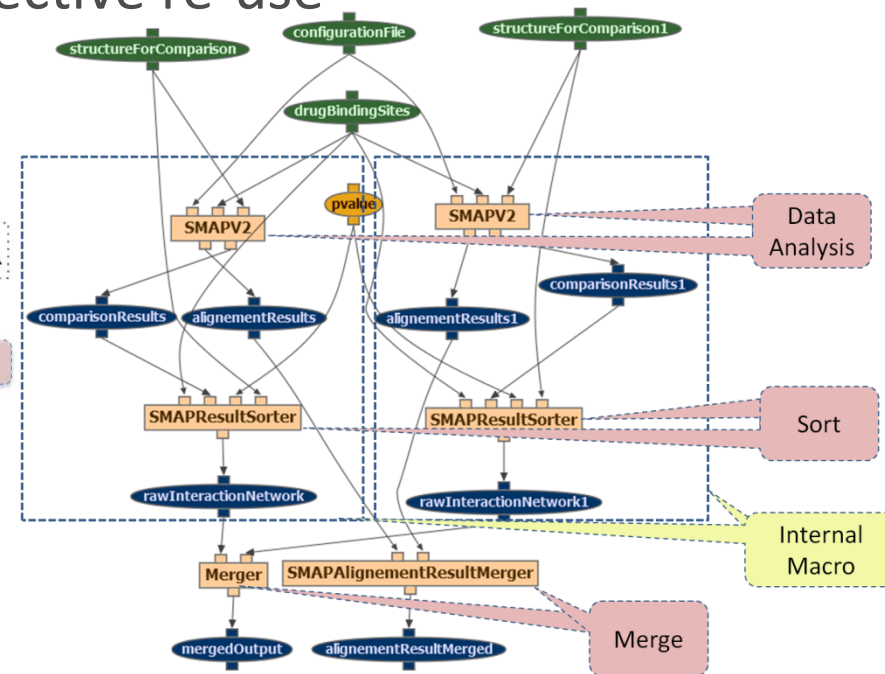
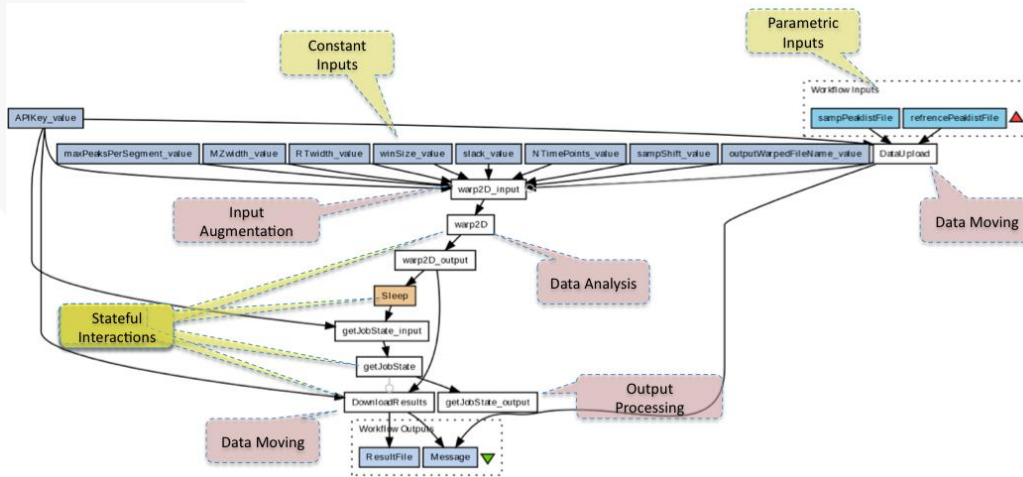
Plan
representation

OPMW

- Empirical analysis on 260 workflow templates from Taverna, Wings, Galaxy and Vistrails
- Catalog of recurring patterns: scientific workflow *motifs*.
 - Data Oriented Motifs
 - Workflow Oriented Motifs
- Understandability and reuse



- Reverse-engineer the set of current practices in workflow development through an analysis of empirical evidence
- Identify workflow abstractions that would facilitate understandability and therefore effective re-use



- Workflow motif: Domain independent **conceptual abstraction** on the workflow steps.

1. Data-oriented motifs: **What** kind of manipulations does the workflow have?

- E.g.:

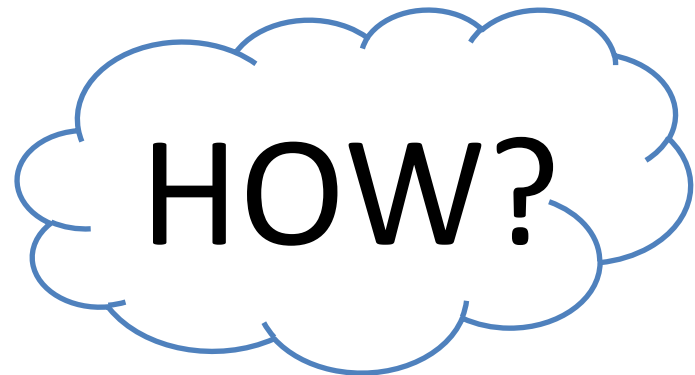
- Data retrieval
- Data preparation
- etc.



2. Workflow-oriented motifs: **How** does the workflow perform its operations?

- E.g.:

- Stateful steps
- Stateless steps
- Human interactions
- etc.



Data-Oriented Motifs

Data Retrieval

Data Preparation

Format Transformation

Input Augmentation
and Output Splitting

Data Organisation

Data Analysis

Data Curation/Cleaning

Data Moving

Data Visualisation

Ontology Purl: <http://purl.org/net/wf-motifs>

Workflow-Oriented Motifs

Intra-Workflow Motifs

Stateful (Asynchronous) Invocations

Stateless (Synchronous) Invocations

Internal Macros

Human Interactions

Inter-Workflow Motifs

Atomic Workflows

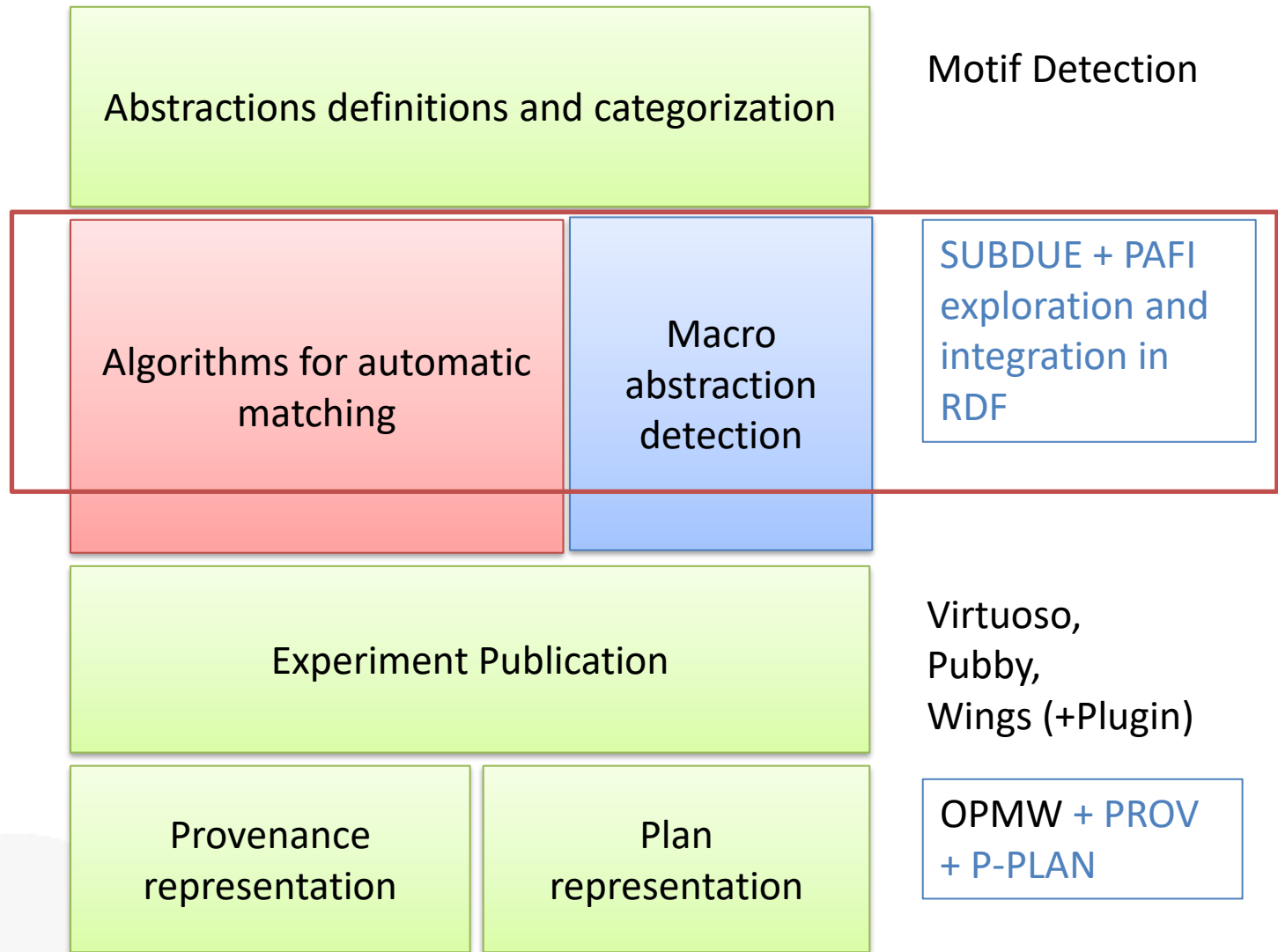
Composite Workflows

Workflow Overloading

Detecting common fragments among scientific workflows (macro motifs)



Detecting common scientific workflow fragments using execution provenance. Garijo, D.; Corcho, O.; and Gil, Y. In *Proceedings of of the seventh international conference on Knowledge capture*, page 33-40, Banff, 2013. ACM.

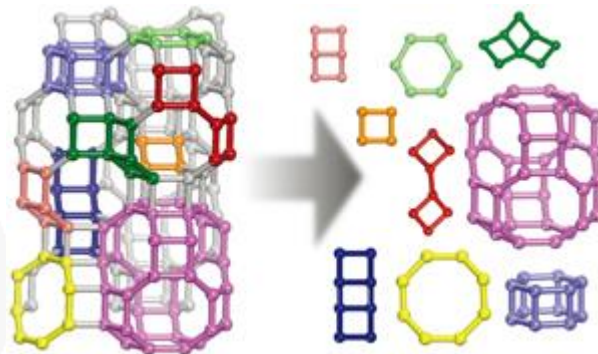


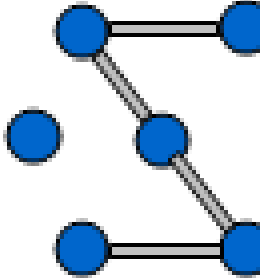
Problem statement:

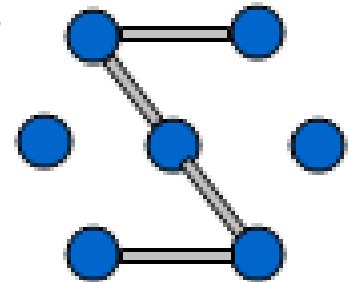
*Given a **repository of workflow templates (either abstract or specific) or workflow execution traces, what are the workflow fragments I can deduce from it?***

Useful for:

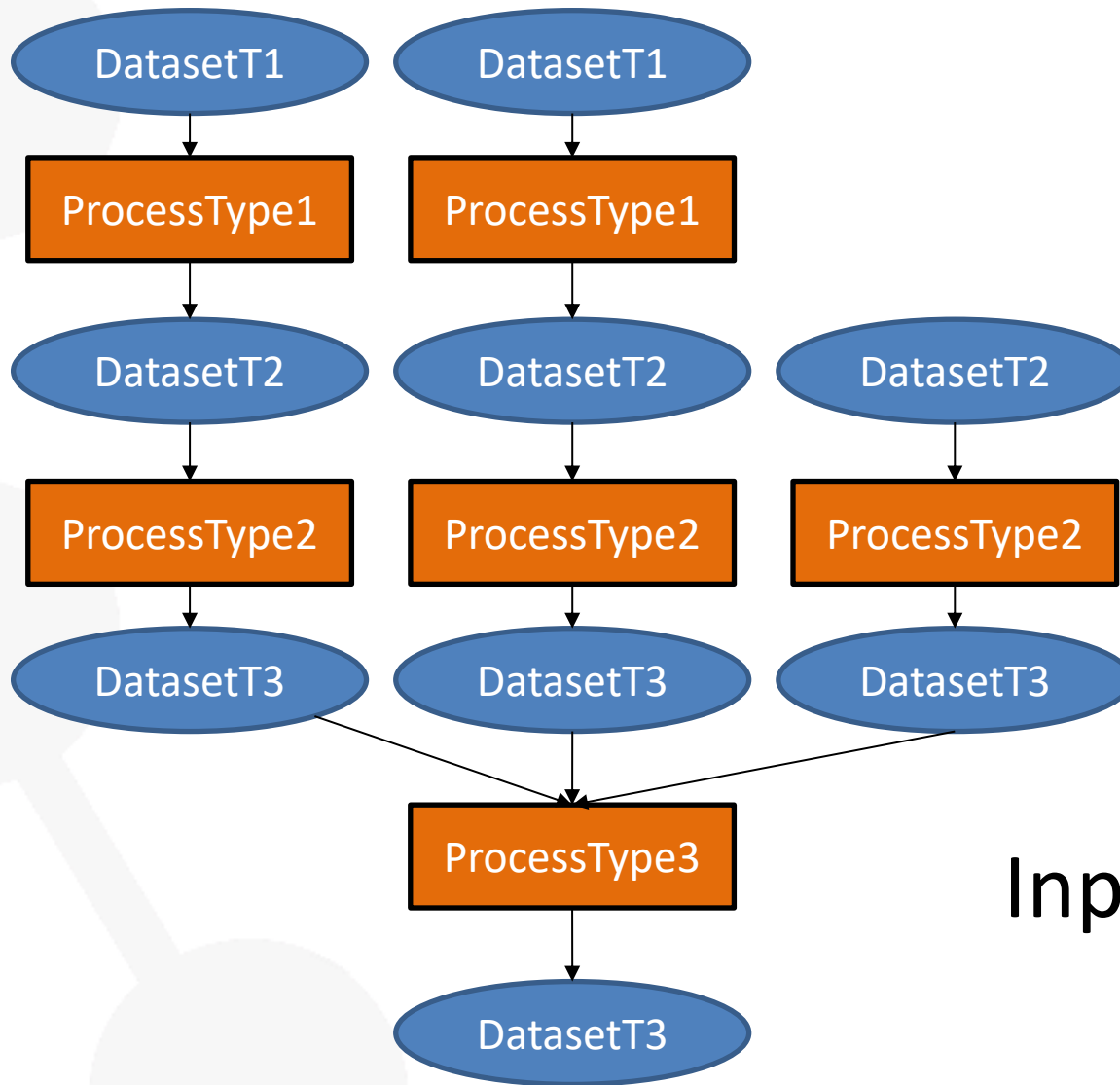
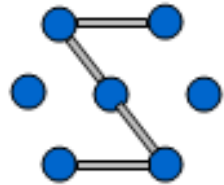
- Systems like [Taverna and Wings](#): (Many templates, little annotation to relate them)
 - Finding relationships between workflows and sub-workflows.
 - Most used fragments, most executed, etc.
- Systems like [GenePattern and Galaxy](#): (Many runs, nearly no templates published)
 - Proposing new templates with the popular fragments.



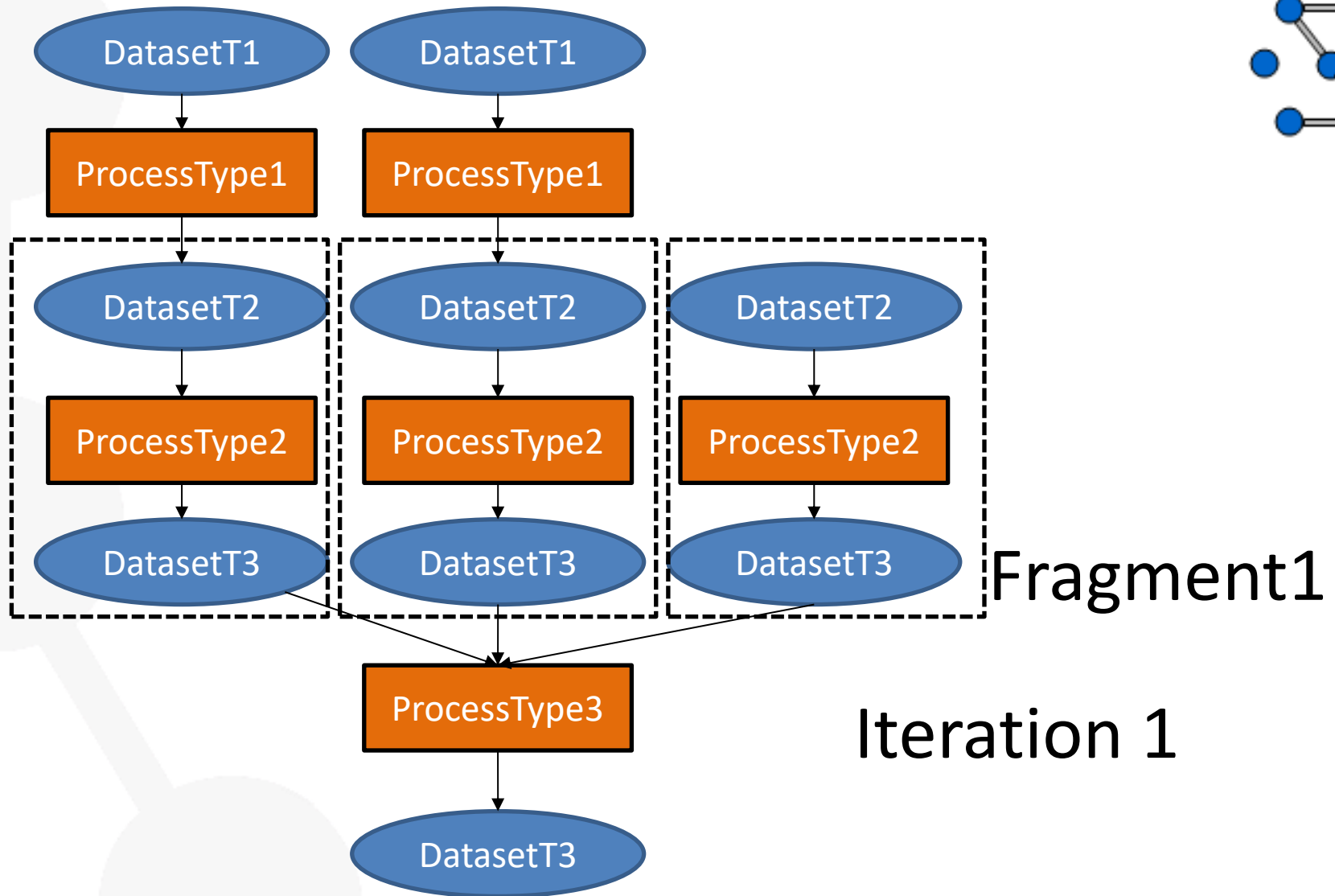
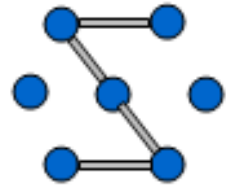
- Given a collection of workflows, which are the **most common fragments**?
 - **Common sub-graphs** among the collection
 - Sub-graph isomorphism (NP-complete)
 - We use the **SUBDUE** algorithm [**Holder et al 1994**] (hierachical clustering)
 - Graph Grammar learning
 - The **rules of the grammar** are the workflow fragments
 - Graph based hierarchical clustering
 - Each **cluster** corresponds to a workflow fragment
 - Iterative algorithm with two measures for compressing the graph:
 - **Minimum Description Length** (MDL)
 - **Size**
 - Current tests with PAFI (<http://glaros.dtc.umn.edu/gkhome/pafi/overview>) ongoing.
- 

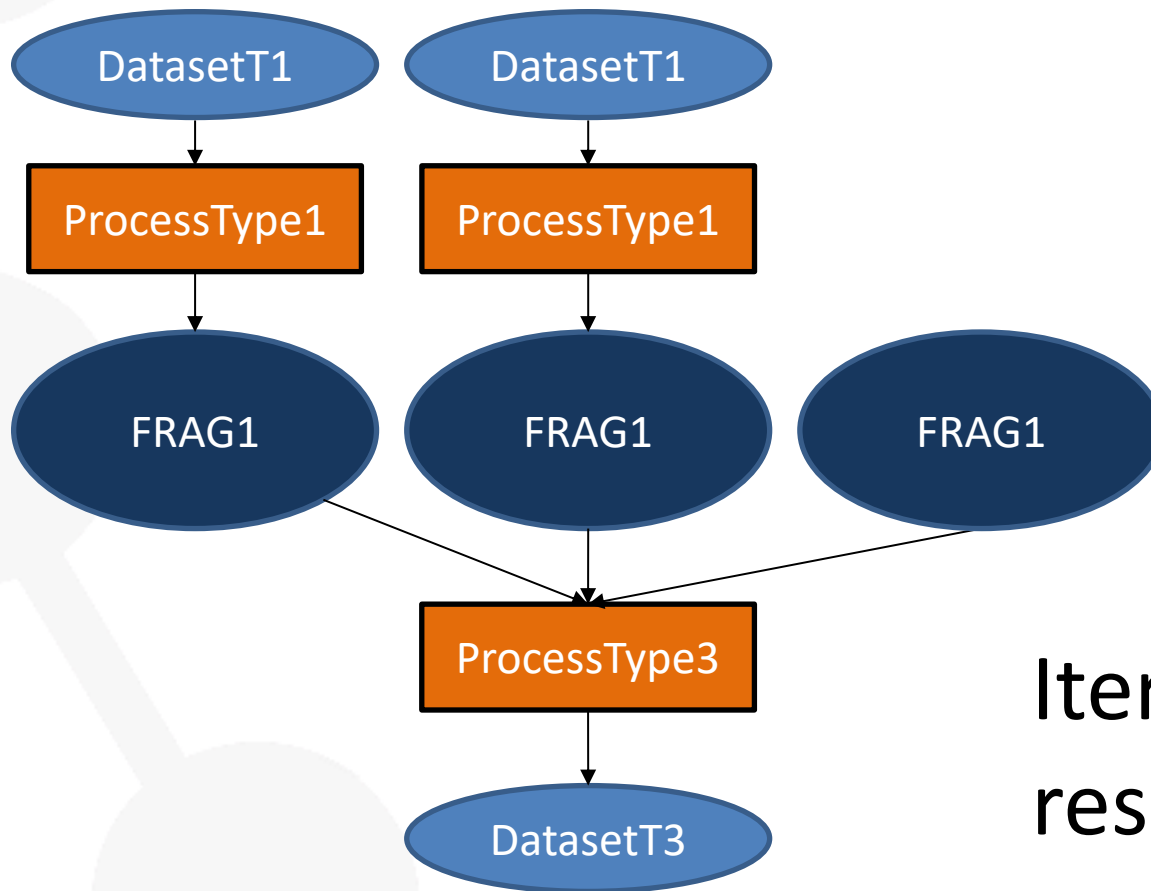
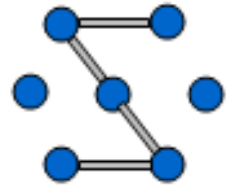


[Holder et al 1994]: **Substructure Discovery in the SUBDUE System** L. B. Holder, D. J. Cook, and S. Djoko. AAAI Workshop on Knowledge Discovery, pages 169-180, 1994.

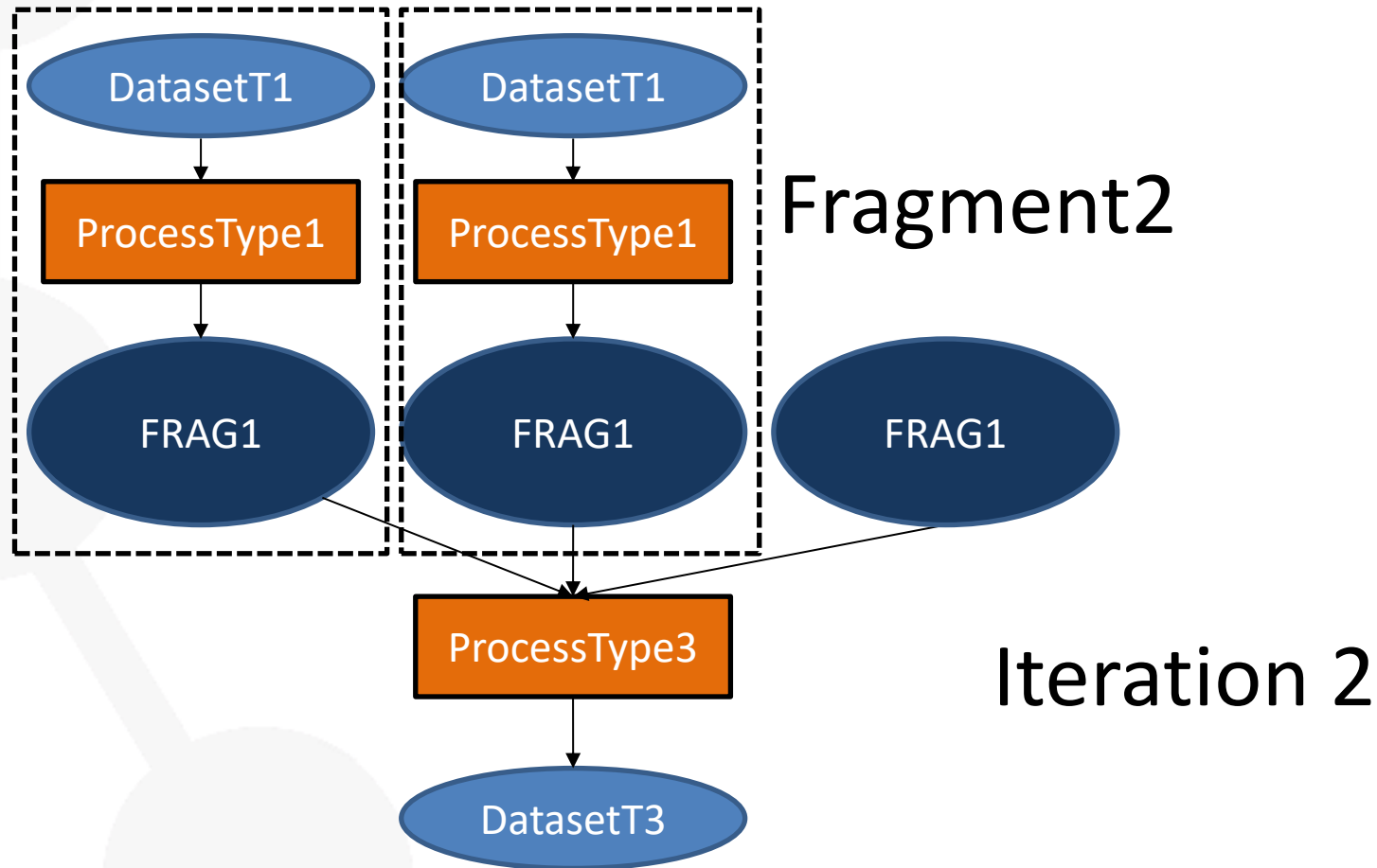
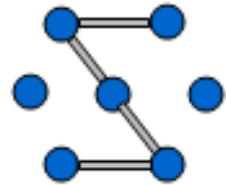


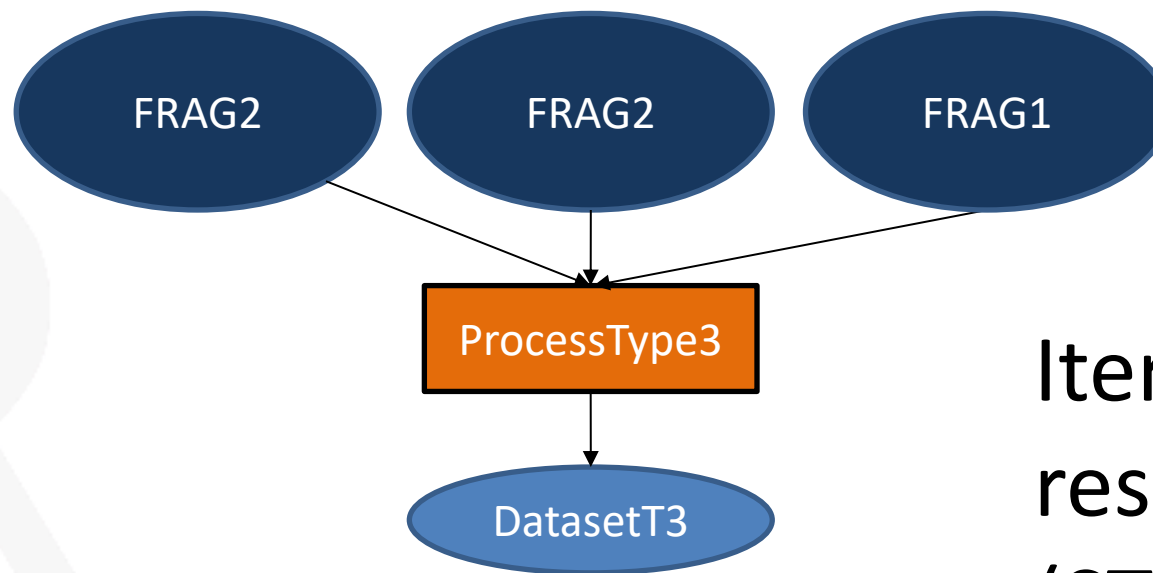
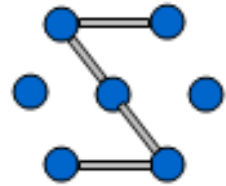
Input Graph



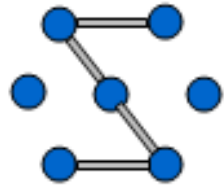


Iteration 1
result



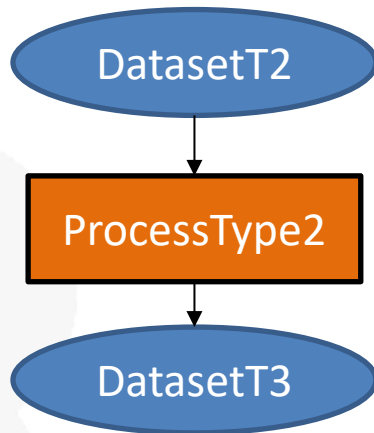


Iteration 2
result
(STOP)



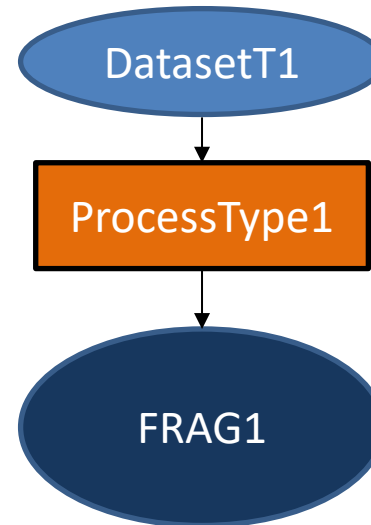
Results:

Fragment 1 (FRAG1) :

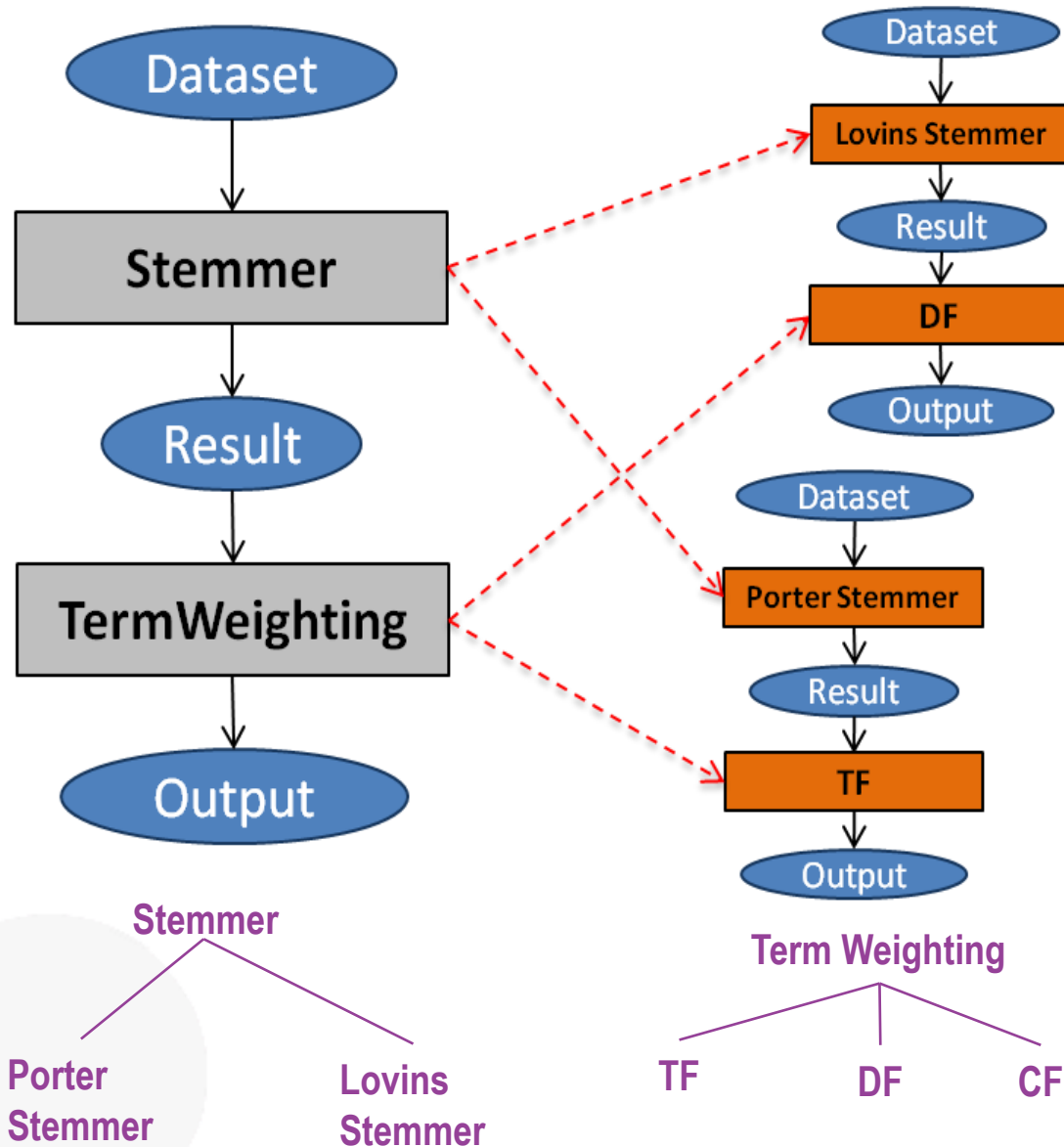


Occurrences:
3 times

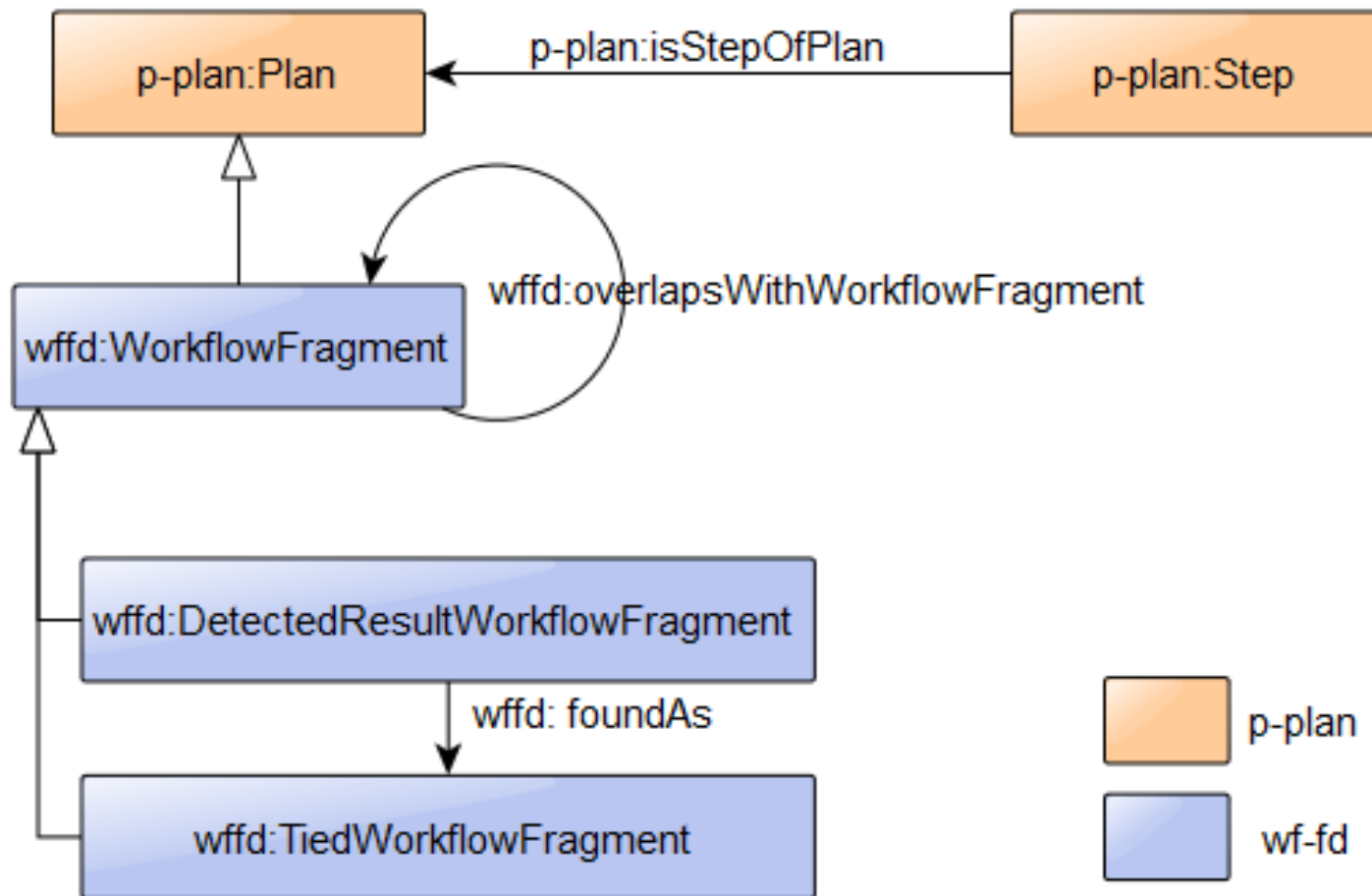
Fragment 2 (FRAG2):



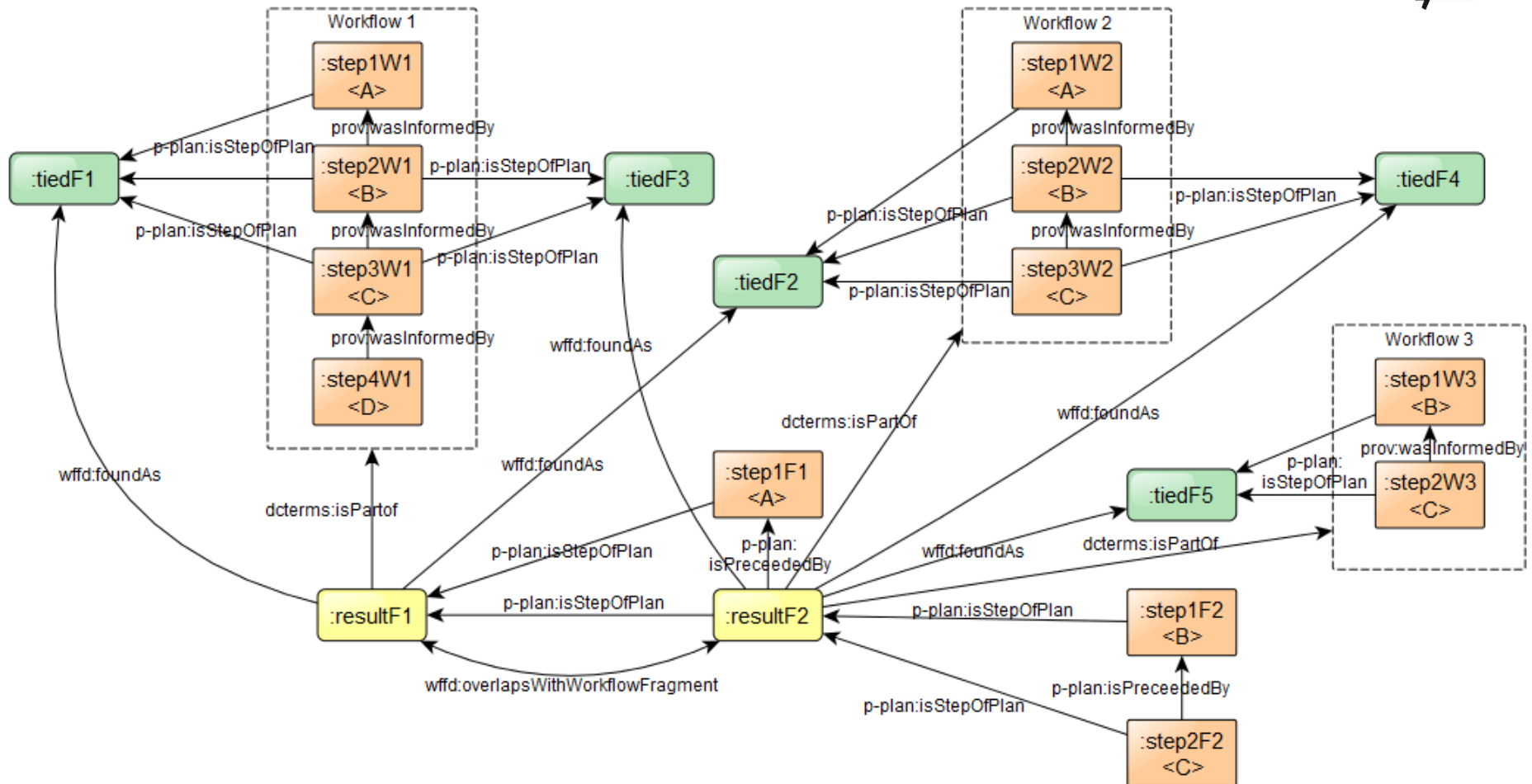
2 times




<http://purl.org/net/wf-fd>



Exporting the fragment results: Wf-FD model



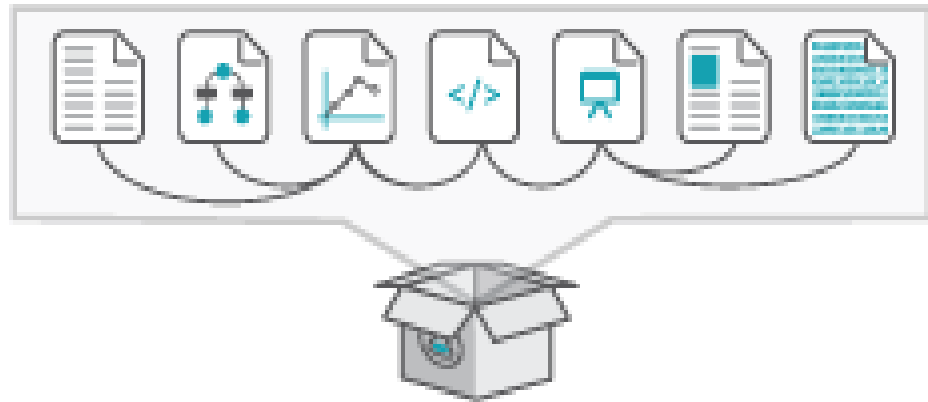
Research Objects

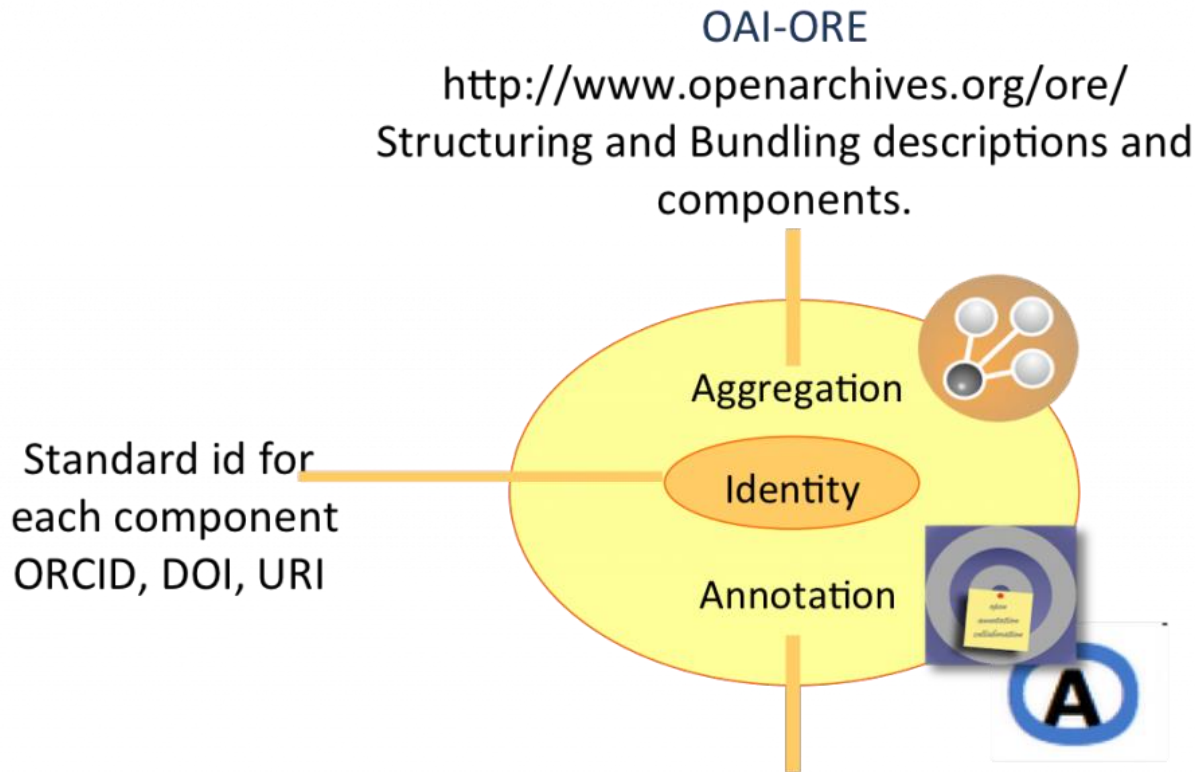


Workflow-Centric Research Objects: First Class Citizens in Scholarly Discourse. Belhajjame, K.; Corcho, O.; Garijo, D.; Zhao, J.; Missier, P.; Newman, D.; Palma, R.; Bechhofer, S.; Garcia, E.; Manuel, .G. J.; Klyne, G.; Page, K.; Roos, M.; Ruiz, J. E.; Soiland-Reyes, S.; Verdes-Montenegro, L.; De Roure, D.; and Goble, C. In *Proceedings of the Second International Conference on the Future of Scholarly Communication and Scientific Publishing Sepublica2012*, page 1-12, Hersonissos, 2012

- Aggregation of resources that bundles together the contents of a research work:

- Data
- Experiments
- Examples
- Bibliography
- Annotations
- Provenance
- ROs
- Etc.





Annotation Data Ontology (AO) + Open Annotation
<http://code.google.com/p/annotation-ontology/>
A generic, domain-neutral annotation framework
<http://www.openannotation.org/spec/core/>

- Tool support
- Interoperability

What can you find in a Research Object? A real example

[Home](#)

[Users](#)

[Groups](#)

[Workflows](#)

[Files](#)

[Packs](#)

[Services](#)

All

[Home](#) > [Packs](#) > [GWAS to pathway](#)

Pack: GWAS to pathway

Created at: 07/02/13 @ 08:32:47

| [Tags \(0\)](#) | [Featured in Packs \(0\)](#) | [Favourited By \(0\)](#) | [Comments \(0\)](#) |

Title: **GWAS to pathway**

Research object: <http://sandbox.wf4ever-project.org/rod/ROs/Pack384/>

Description

This pack is for a workflow that finds KEGG pathways for genes from a GWAS.

Uploaded by

- [Stian Soiland-Reyes](#) (last uploaded on 2012-12-24 18:40)
- [Khalid Belhajjame](#) (last uploaded on 2012-11-02 18:40)

Authors

- [Kristina Hettne](#) (last authored on 2012-12-24 18:40)
- [Marco Roos](#) (last authored on 2012-10-15 11:24)

Contributors

Creator



[Marco Roos](#)

6 items in this pack

Navigate RO

- root
 - biblio/
 - produced/
 - used/
 - config/
 - scripts/
 - setup/
 - software/
 - web services/

New/Upload

Pack



[Stian Soiland-Reyes](#)

- [My Profile](#) [edit]
- [My Messages \(3\)](#)
- [My Memberships](#)
- [My History](#)
- [My News](#)

3 new messages

- [RE: hehe..](#)
- [RE: Hello](#)
- [RE: testing](#)

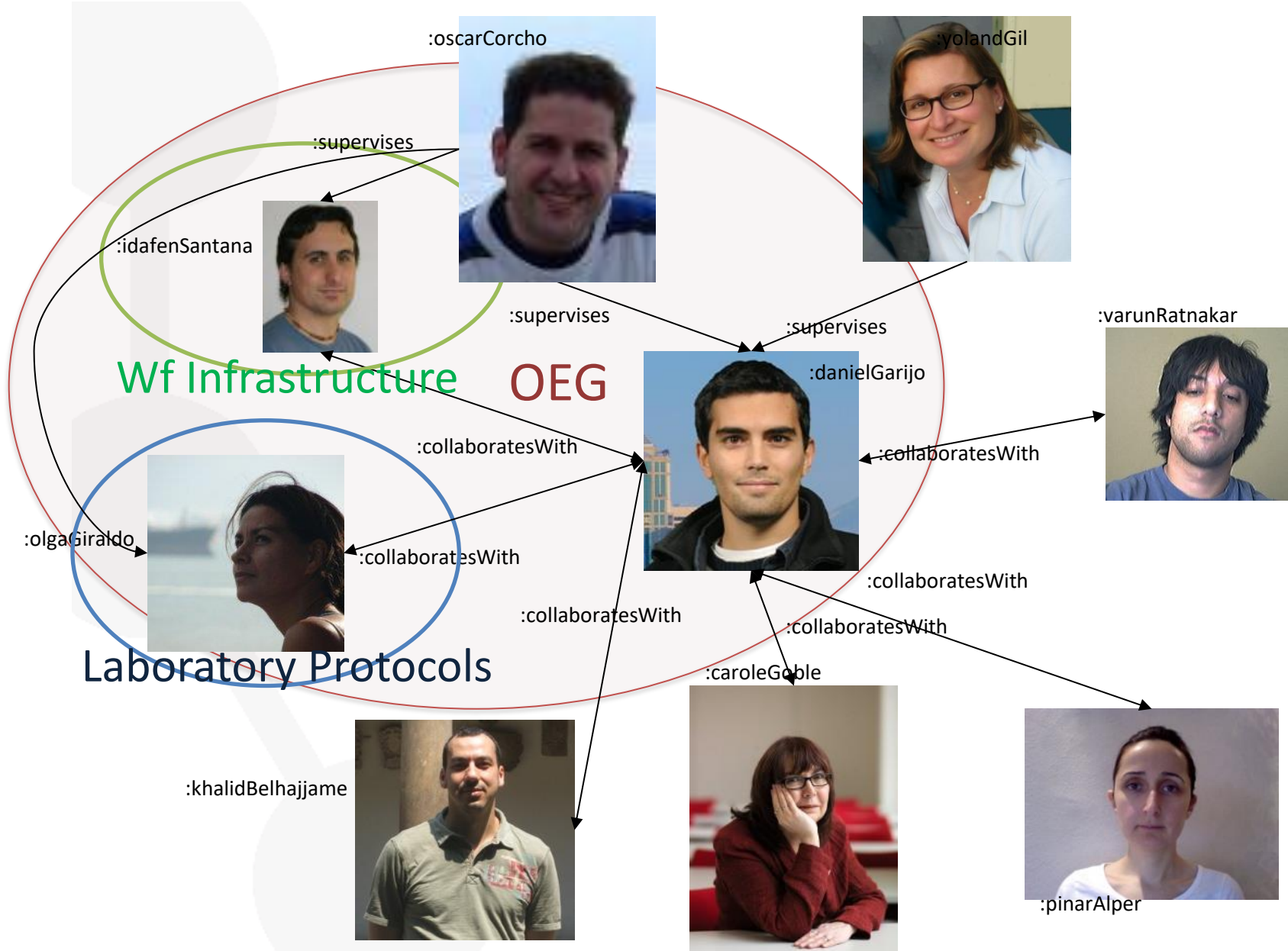
1 new friendship request

- [Raul Palma](#)

My Stuff

[21 Friends](#) | [5 Groups](#) | [47 Workflows](#) | [17 Packs](#)

- Finish integrating some other graph algorithms
 - PAFI (almost done)
 - Parsemis
- Test other workflow systems
 - LONI (from ISI)
 - GenePattern/Galaxy?
- Build a corpus for evaluation
 - Gold standard to test the different results.
- Perform evaluation
 - Analyze which is the best way to characterize the fragments
 - Presentation of the results
- Write paper(s)





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