Janus:
from Workflows to Semantic Provenance and Linked Open Data

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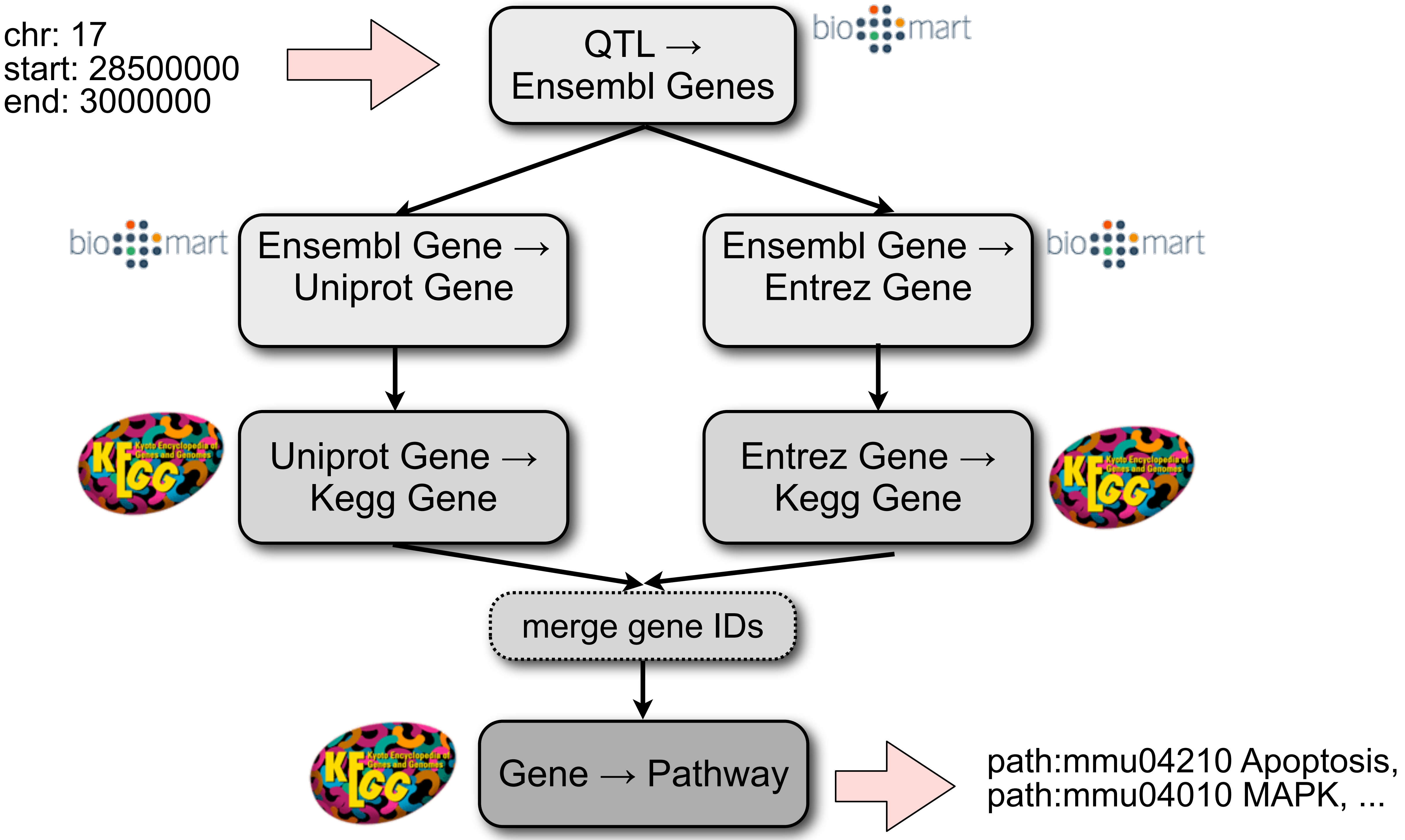
Key ideas

- Janus:
  - a semantic provenance model with domain-specific extensions
  - designed around the Taverna workflow model
- From domain-agnostic provenance graphs
- To domain-aware graphs through explicit annotations
- From local provenance graphs and queries scoped to the graph
- To
  - Graphs published as Linked Data
  - Queries extended into the Web of Data

Example workflow (Taverna)



chr: 17
start: 28500000
end: 3000000

QTL → Ensembl Genes

Ensembl Gene → Uniprot Gene

Ensembl Gene → Entrez Gene

Uniprot Gene → Kegg Gene

Entrez Gene → Kegg Gene

merge gene IDs

Gene → Pathway

path:mmu04210 Apoptosis,
path:mmu04010 MAPK, ...

biomart
biomart
biomart
KEGG Kyoto Encyclopedia of Genes and Genomes
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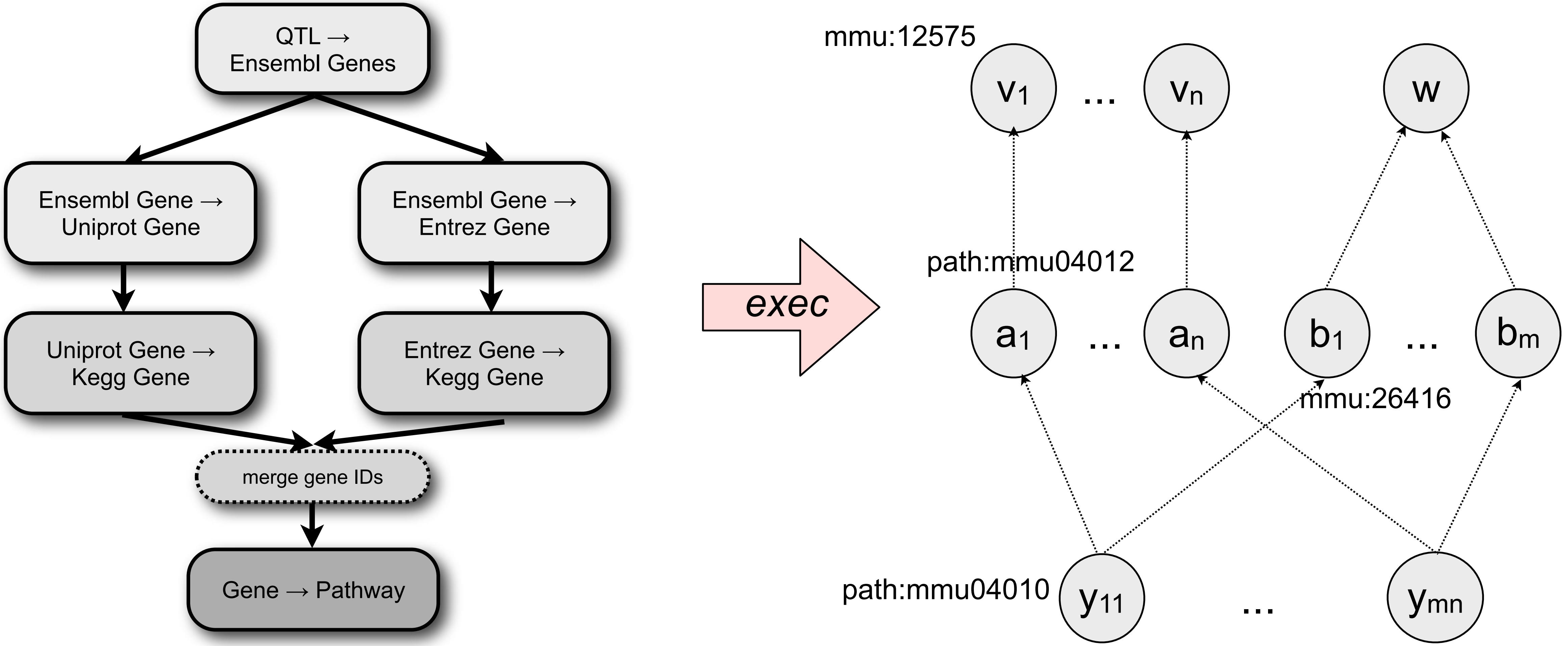
Baseline provenance of a workflow run

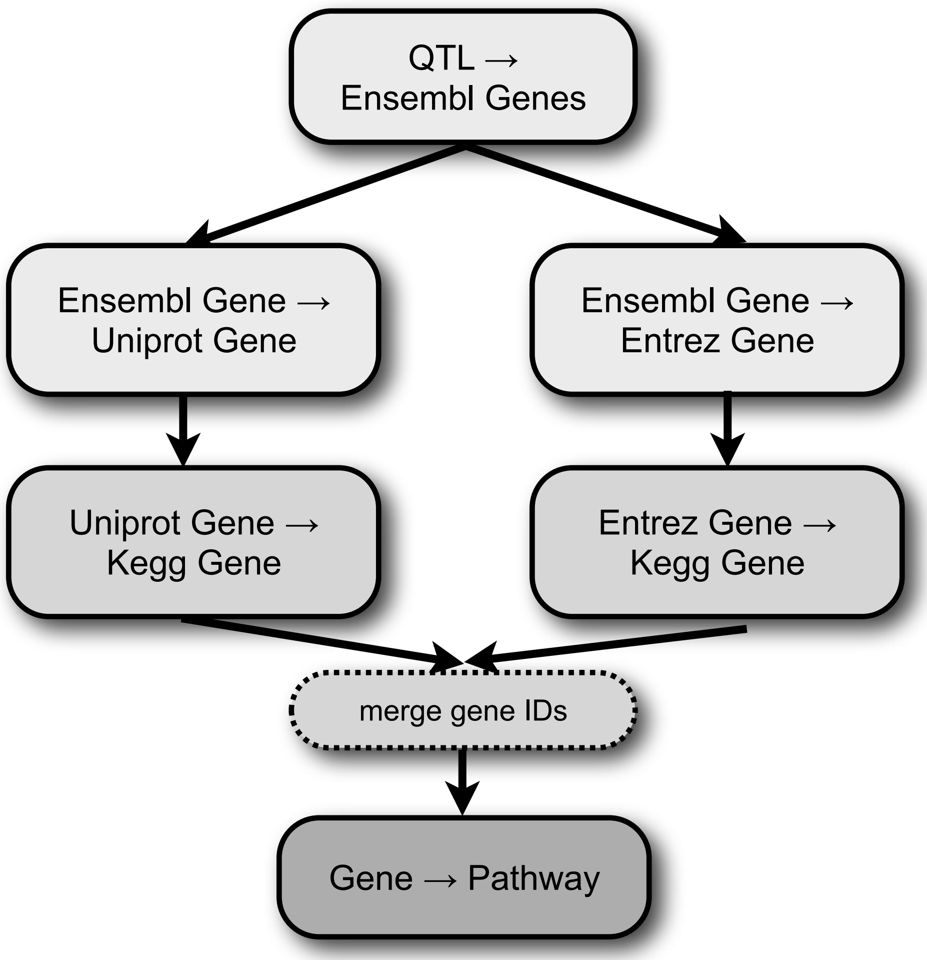


path:mmu04010→*derives_from*→mmu:26416

path:mmu04012→*derives_from*→mmu:12575

- The graph encodes all direct data dependency relations
- Baseline query model: compute paths amongst sets of nodes
  - Transitive closure over data dependency relations

Reference user questions



Q0: Find all intermediate and initial input values that contribute to the computation of a certain output value.

Q1. Find all those genes within the input QTL region that are involved in a given KEGG pathway.

Q2: Find all Uniprot-sourced genes

Q3: Find all Entrez genes that encode proteins involved in ATP binding (go: 0005524).

Q4: List relevant PubMed publications for the pathways listed in the result set.

Query types and model capabilities

	Query formulation effort	Annotation requirements	Query Scope
Q0	- Requires knowledge of process structure and data values - Graphical query constructor may be available	No annotations required	Single run graph or Multi-run graphs
Q1 Q2	Use of domain terms facilitates query formulation	Requires domain annotations on workflow tasks and on data values	Single run graph or Multi-run graphs
Q3 Q4	- Use of domain terms facilitates query formulation. - Can be integrated with browsers for LoD sources	- Requires domain annotations on workflow tasks and on data values - Relies on completeness of Linked Data Sources	The Web of Data

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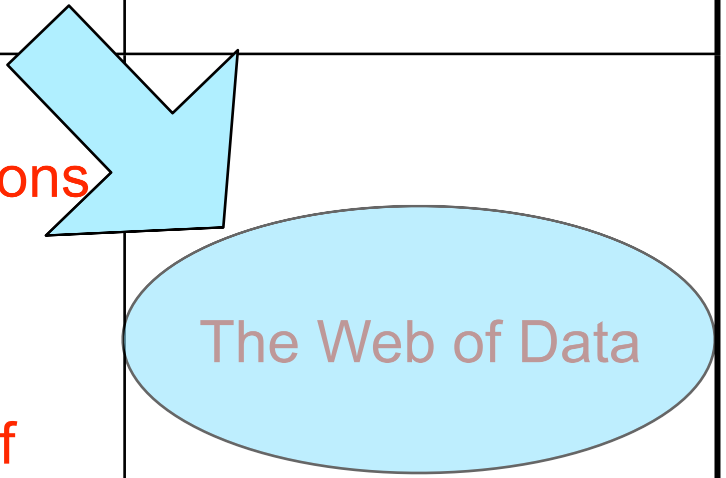
Q3 Q4	- Use of domain terms facilitates query formulation. - Can be integrated with browsers for LoD sources	- Requires domain annotations on workflow tasks and on data values - Relies on completeness of Linked Data Sources	 The Web of Data

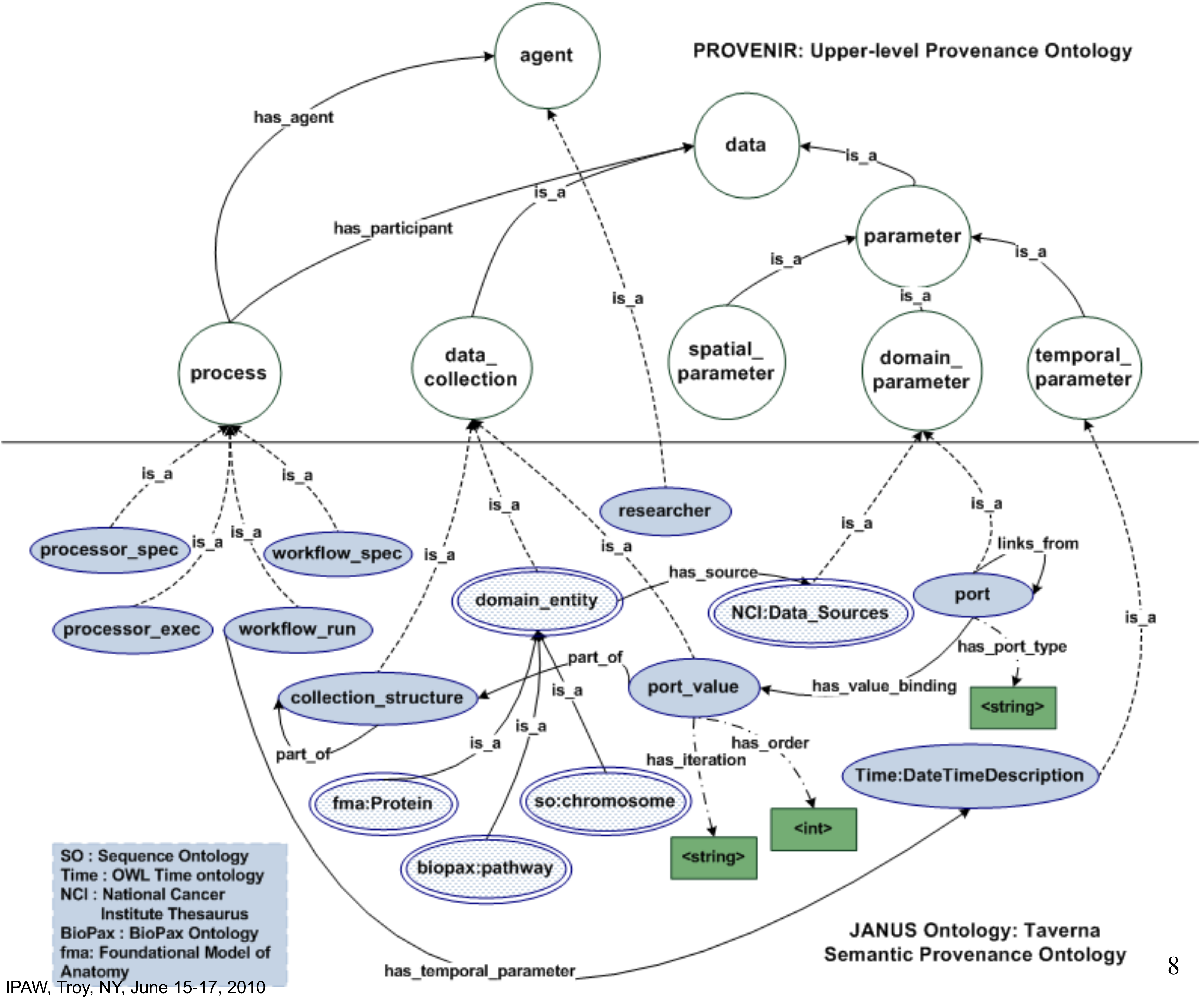
Janus: baseline model of provenance

- The semantic provenance model is an OWL ontology
  - defined for domain-agnostic provenance graphs
  - naturally extensible to domain concepts

- extends the Provenir upper ontology [*]
  - Itself an extension of the Basic Formal Ontology (BFO)
    - abstract concepts include *data*, *process*, and *agent*
  - Provenir adds 11 types of relationships:
    - partonomy relations
    - temporal information
    - precedence
    - causal relationships
    - ...

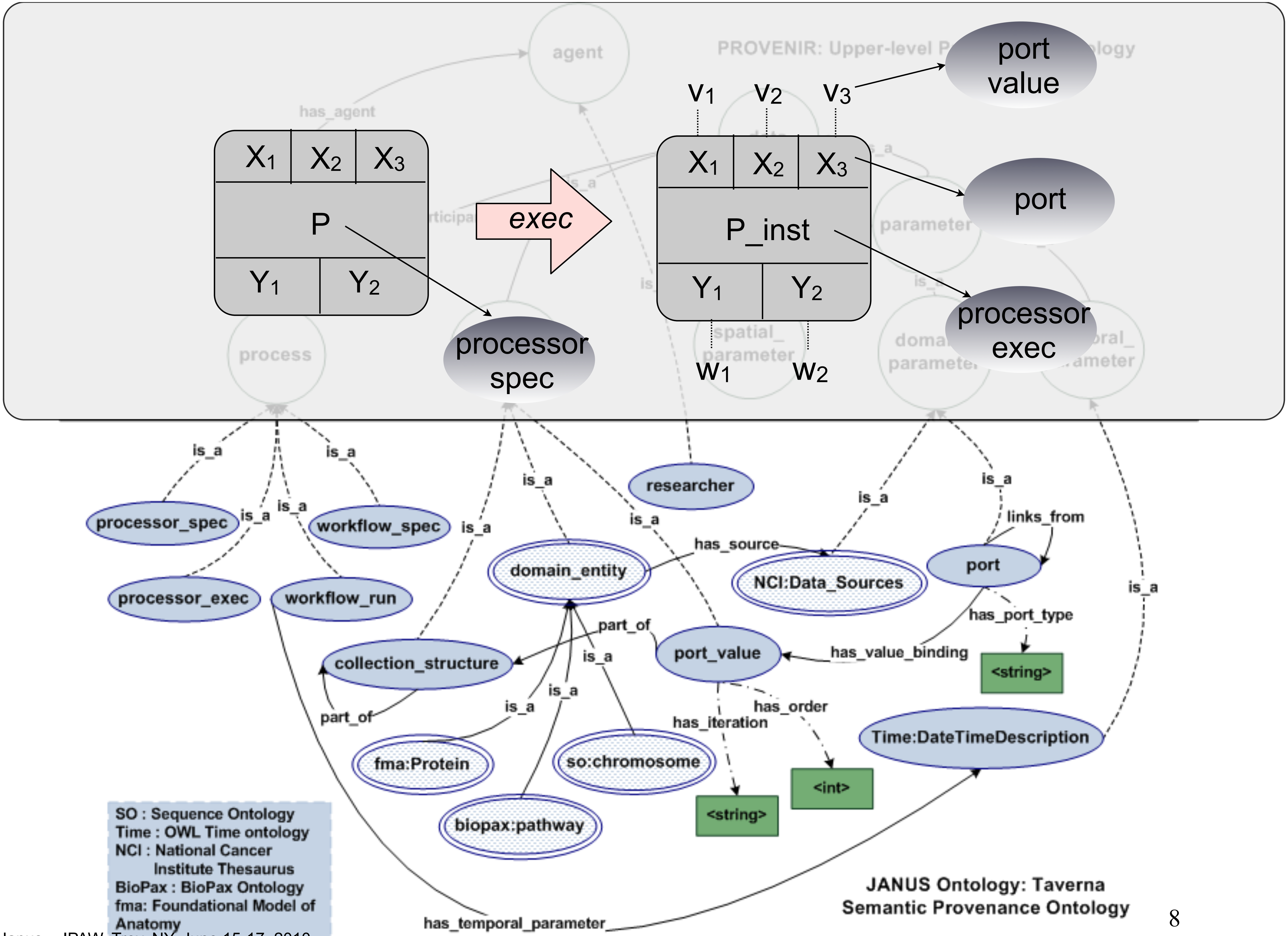
[*] S. Sahoo and A. Sheth. Provenir ontology: Towards a Framework for eScience Provenance Management, Knoesis Center Tech Report, 2009.

Janus structure



SO : Sequence Ontology
Time : OWL Time ontology
NCI : National Cancer Institute Thesaurus
BioPax : BioPax Ontology
fma: Foundational Model of Anatomy

Janus structure



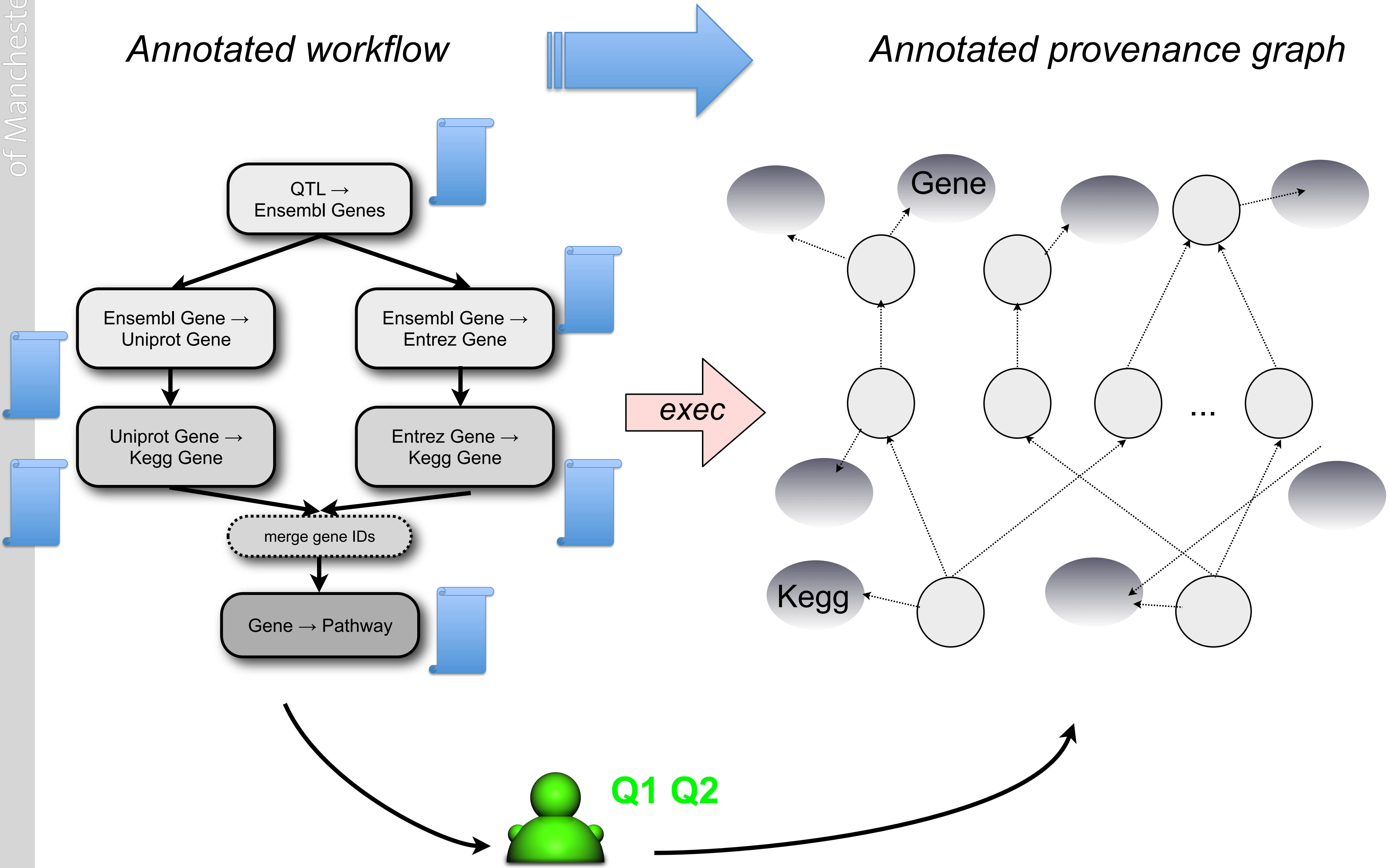
Example Janus domain-agnostic fragment

```
<rdf:Description rdf:about="http://purl.org/net/taverna/janus/remove_Nulls">
<janus:has_execution rdf:resource="http://purl.org/net/taverna/janus/remove_Nulls"/>
<knoesis:has_parameter rdf:resource="http://purl.org/net/taverna/janus/remove_Nulls/output"/>
<knoesis:has_parameter rdf:resource="http://purl.org/net/taverna/janus/remove_Nulls/input"/>
<obo:part_of rdf:resource="http://purl.org/net/taverna/janus/e589d90b-01f2-4de6-..."/>
<rdf:type rdf:resource="http://purl.org/net/taverna/janus#processor_spec"/>


<rdf:Description rdf:about="http://purl.org/net/taverna/janus/remove_Nulls/input">
<janus:has_value_binding rdf:resource="http://purl.org/net/taverna/janus/test1625"/>
<janus:links_from rdf:resource="http://purl.org/net/taverna/janus/merge_entrez_genes/
concatenated"/>
<janus:is_processor_input rdf:datatype="http://www.w3.org/2001/
XMLSchema#boolean">true</janus:is_processor_input>
<rdf:type rdf:resource="http://purl.org/net/taverna/janus#port"/>


<rdf:Description rdf:about="http://purl.org/net/taverna/janus/test1625">
<janus:has_iteration rdf:datatype="http://www.w3.org/2001/XMLSchema#string">[]</
janus:has_iteration>
<rdf:type rdf:resource="http://purl.org/net/taverna/janus#port_value"/>
</rdf:Description>
```

Annotated provenance



Annotated workflow

Annotated provenance graph

QTL → Ensembl Genes

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merge gene IDs

Gene → Pathway

exec

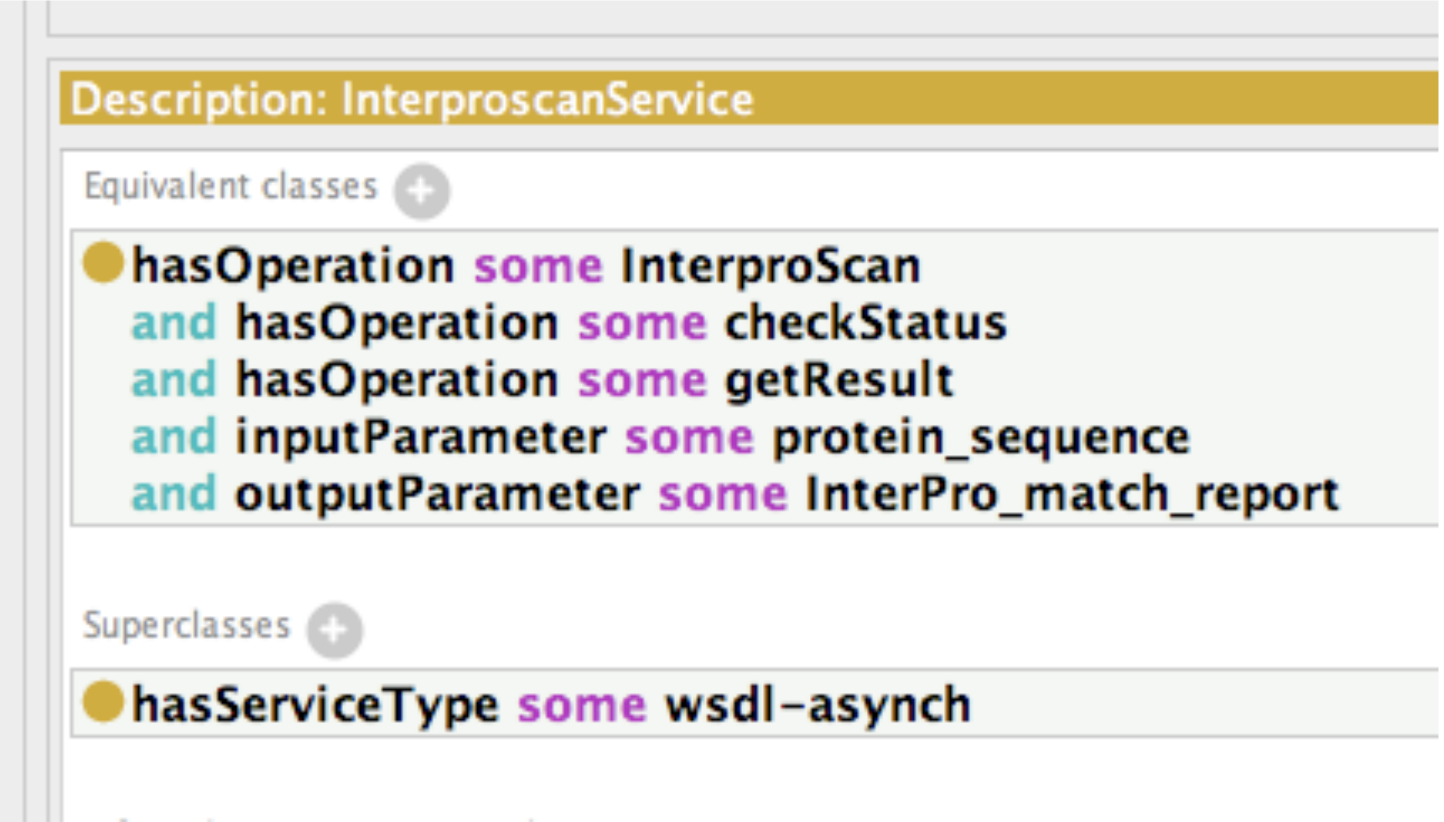
Gene

Kegg

…

Q1 Q2

Desiderata: from structure to values annotations



Description: InterproscanService

Equivalent classes

● hasOperation some InterproScan
and hasOperation some checkStatus
and hasOperation some getResult
and inputParameter some protein_sequence
and outputParameter some InterPro_match_report

Superclasses

● hasServiceType some wsdl-asynch

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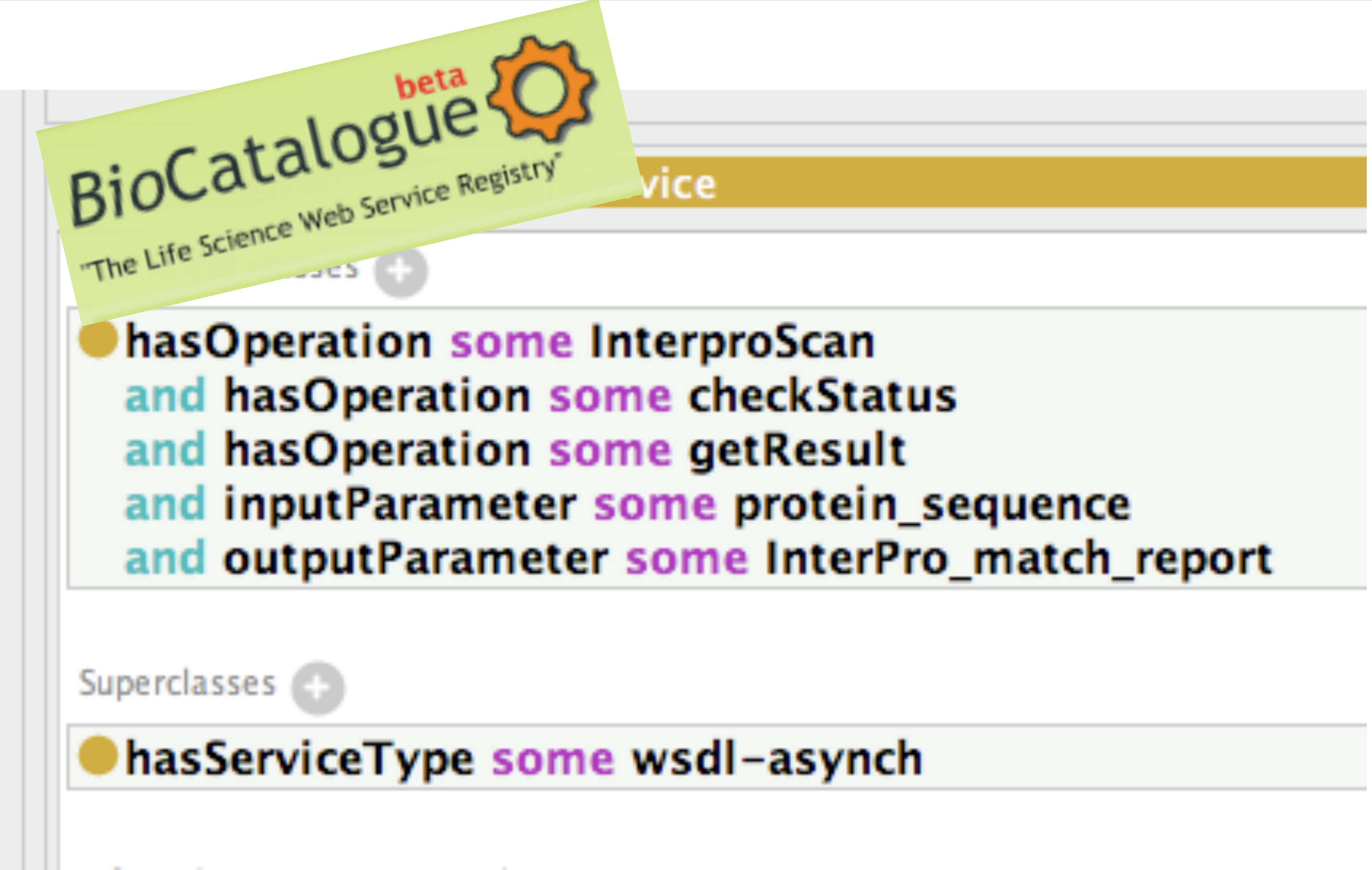

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Superclasses

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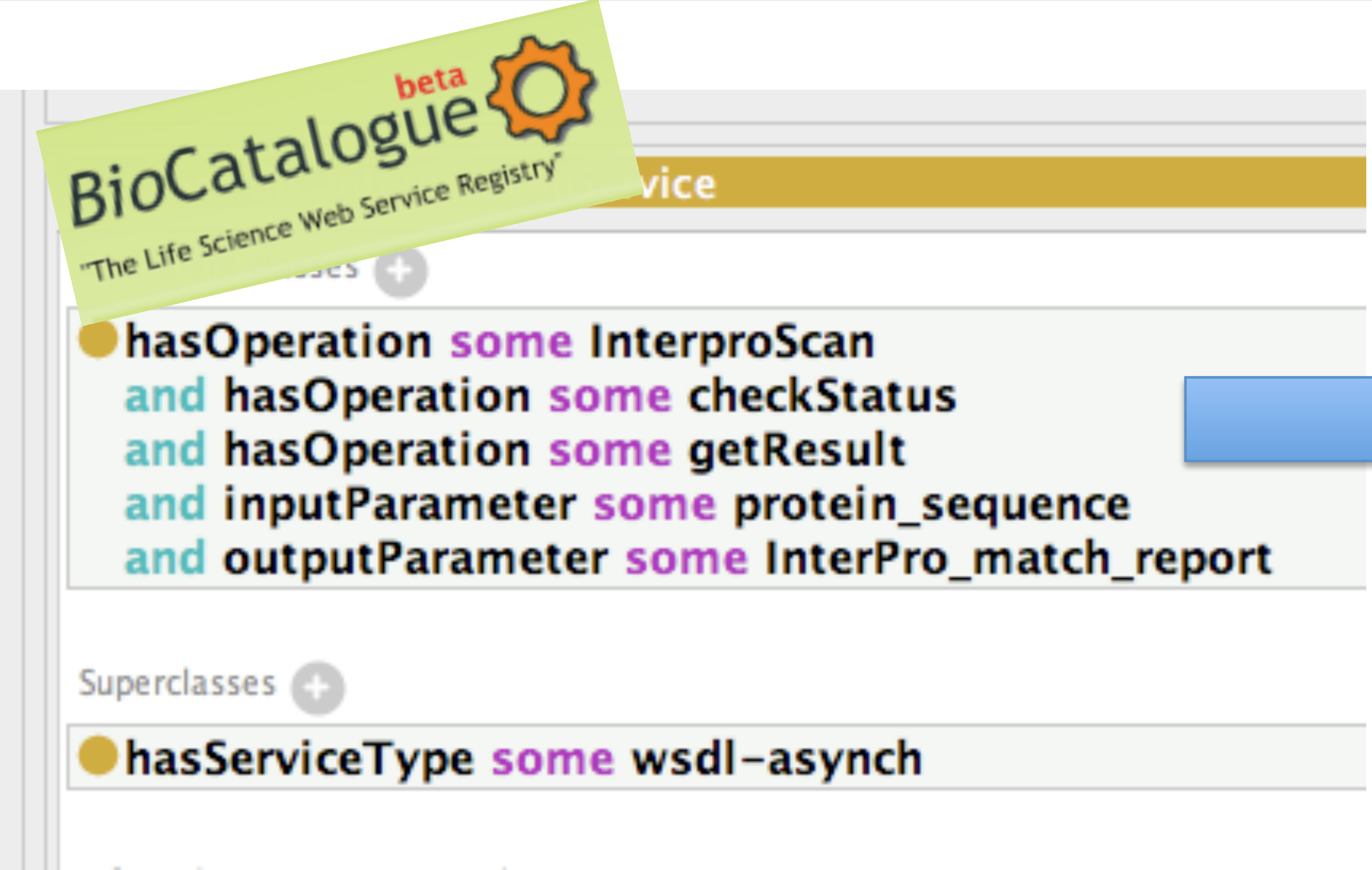

BioCatalogue beta

"The Life Science Web Service Registry"

hasOperation some InterproScan
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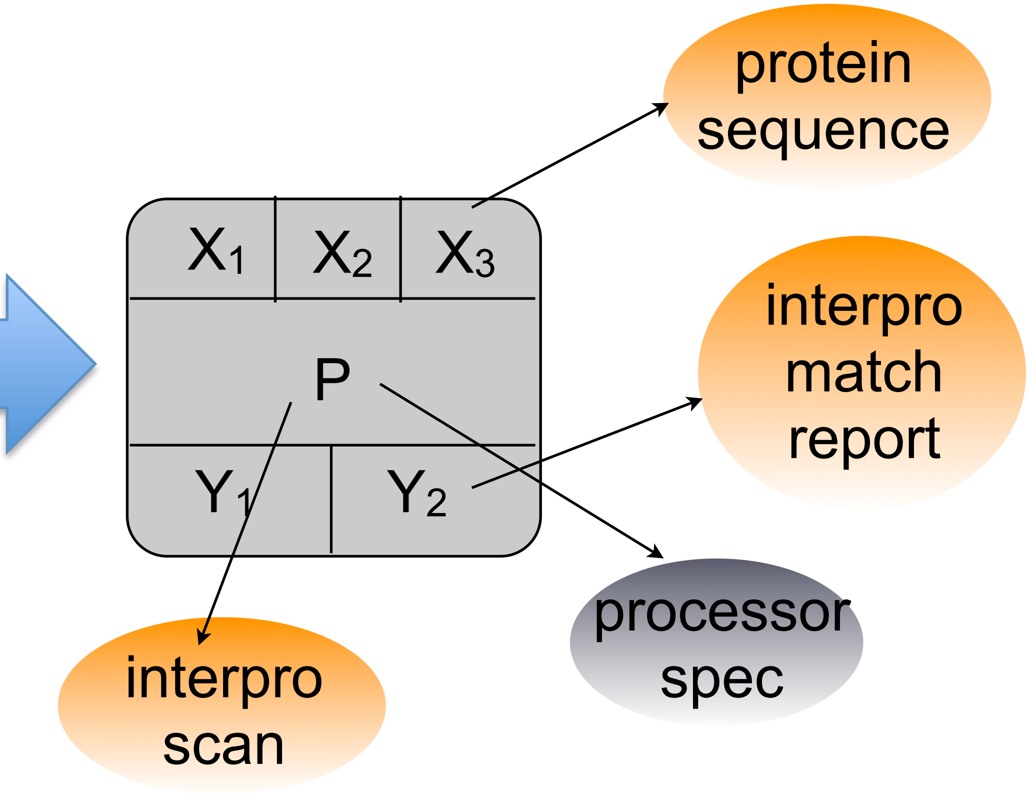
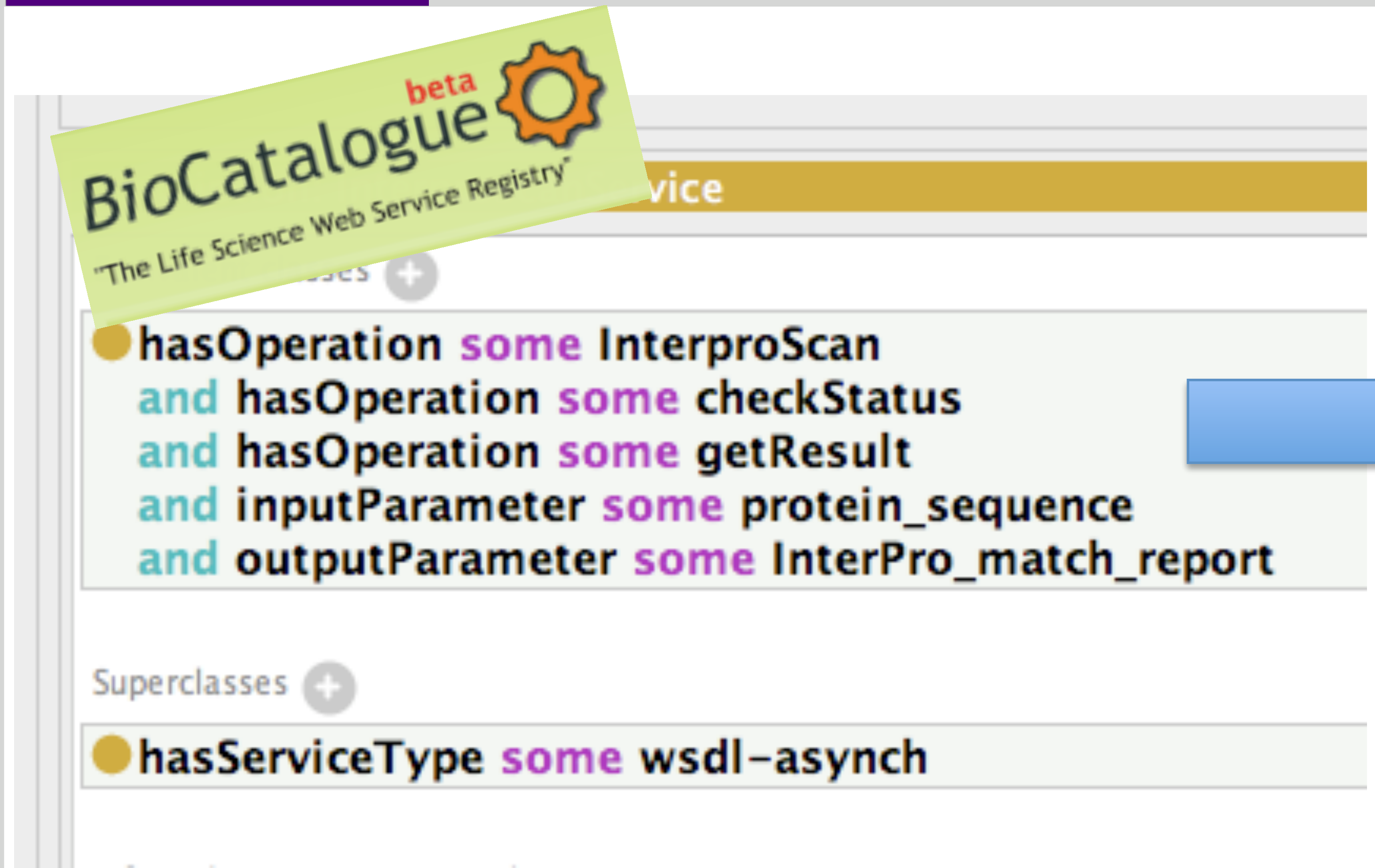


Desiderata: from structure to values annotations



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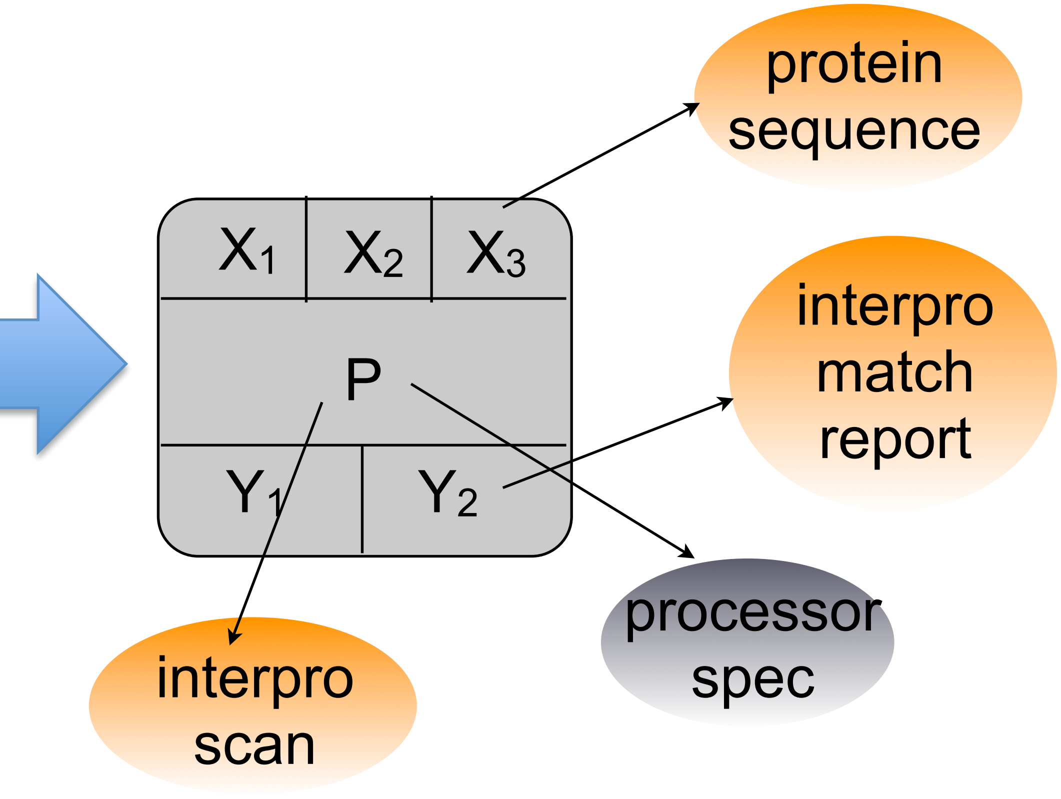
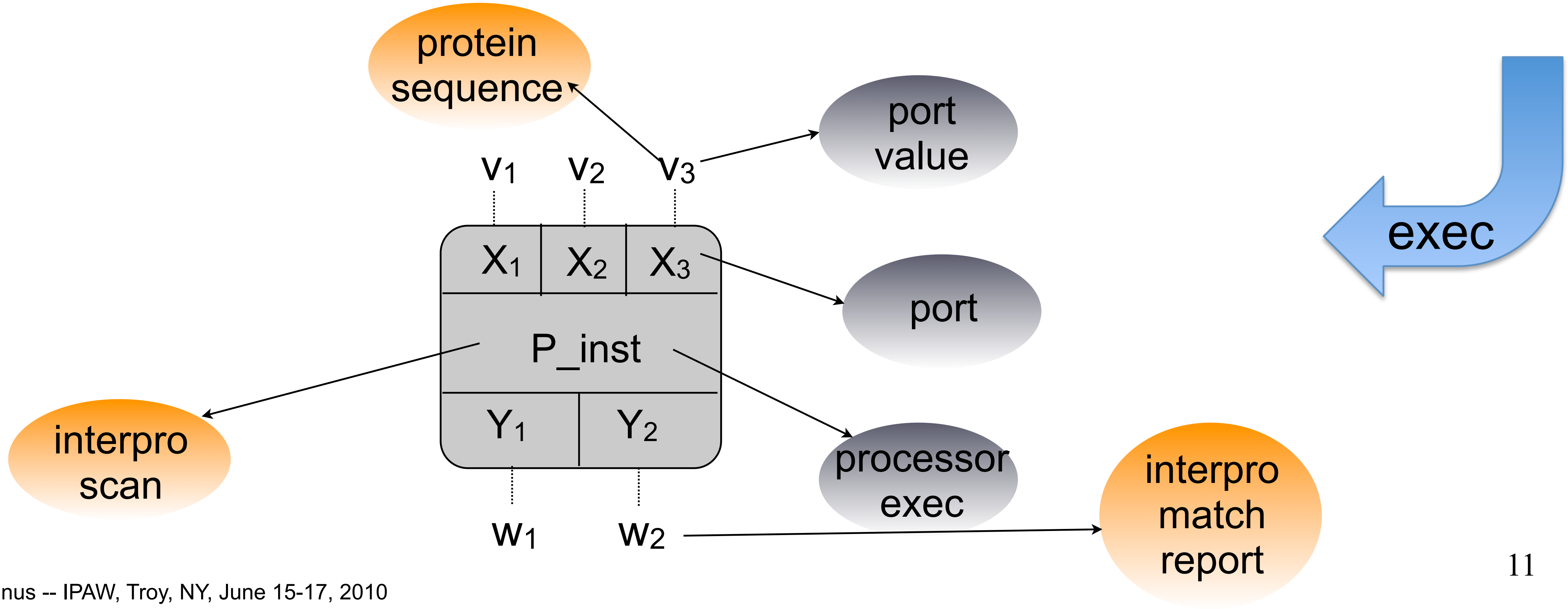


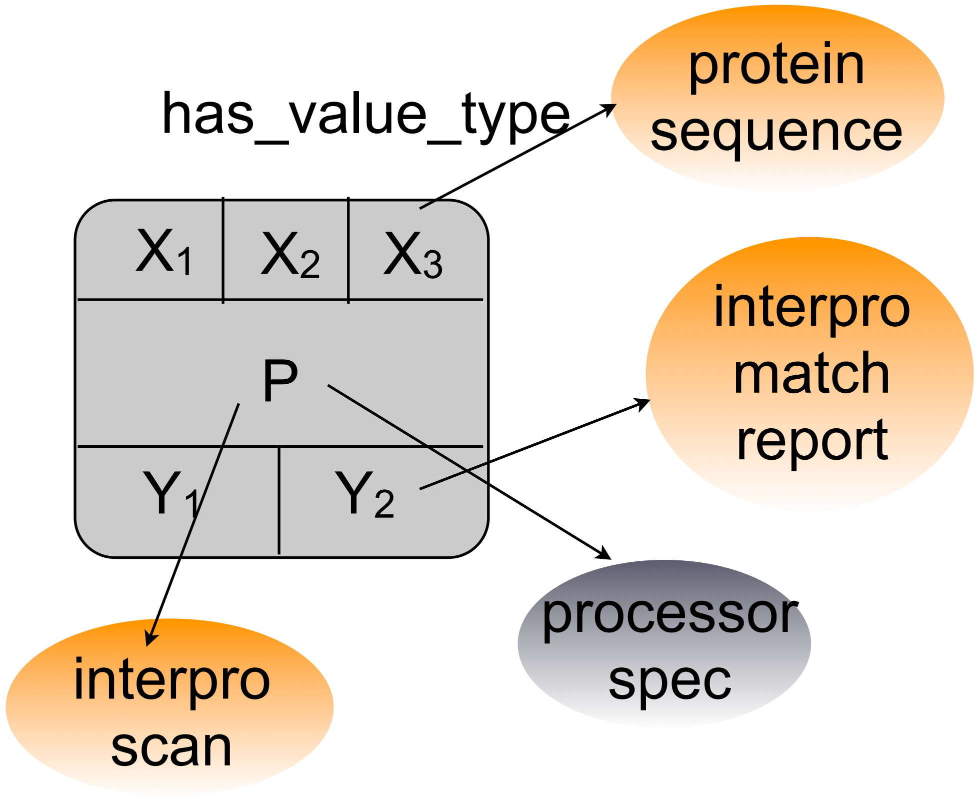


MANCHESTER 1824

Annotations propagation rules

$$\frac{X\ \texttt{rdf:type Port} \qquad C = \{c\} \qquad X\ \texttt{has\_value\_type}\ c \qquad X\ \texttt{has\_value}\ v \qquad v\ \texttt{rdf:type PortValue}}{v\ \texttt{rdf:type}\ C}$$

denotes data type in the PL sense



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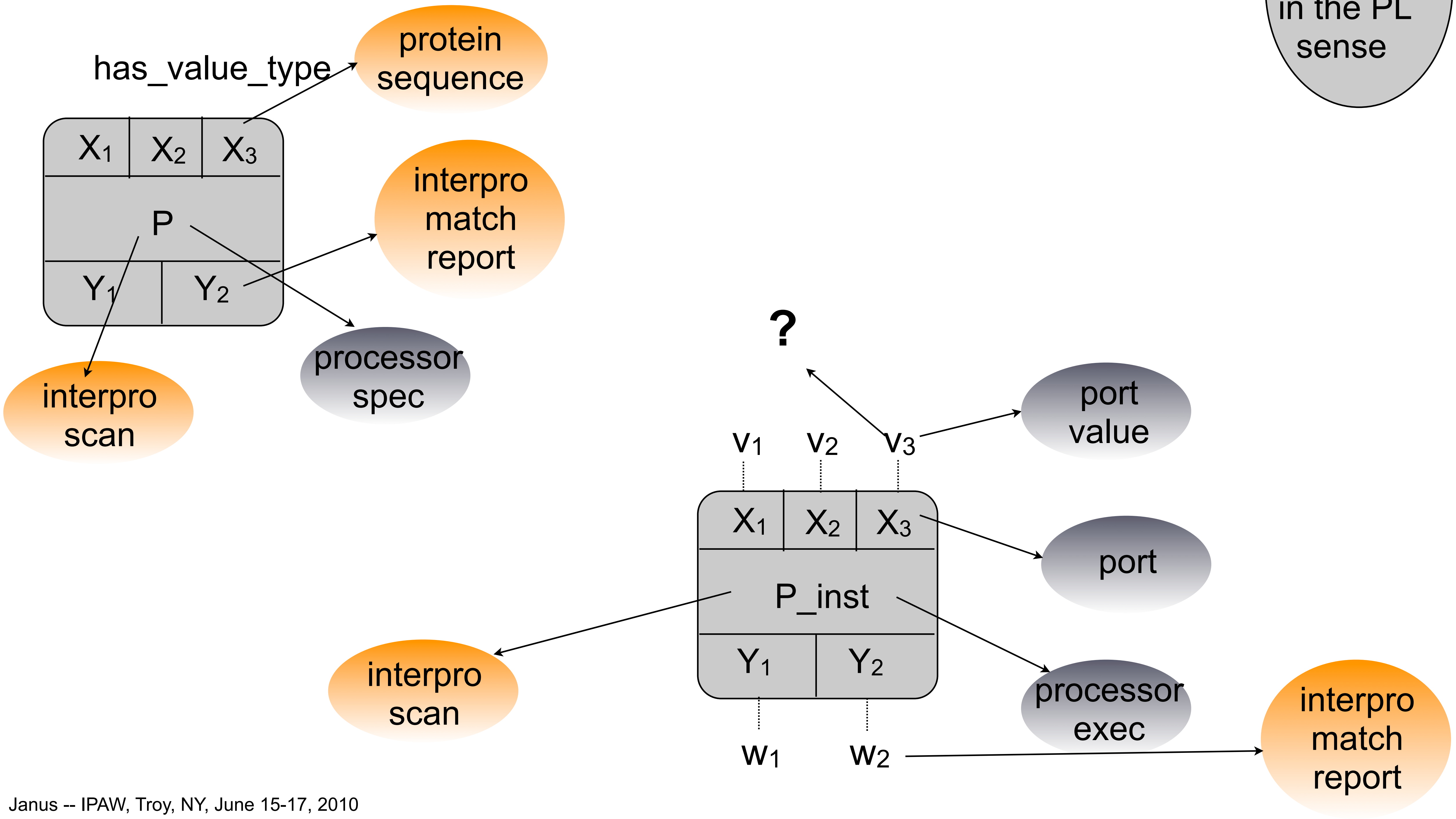

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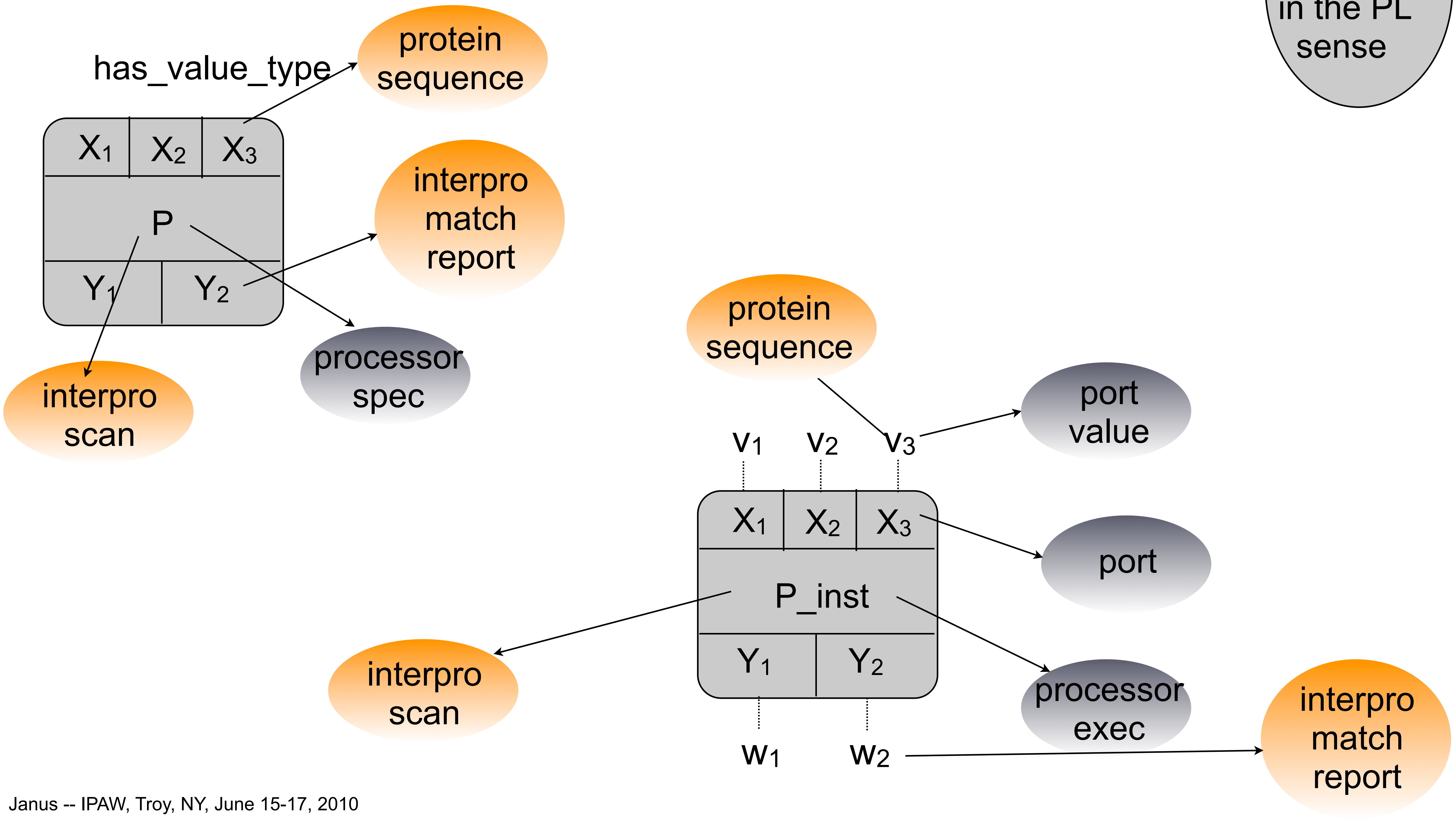
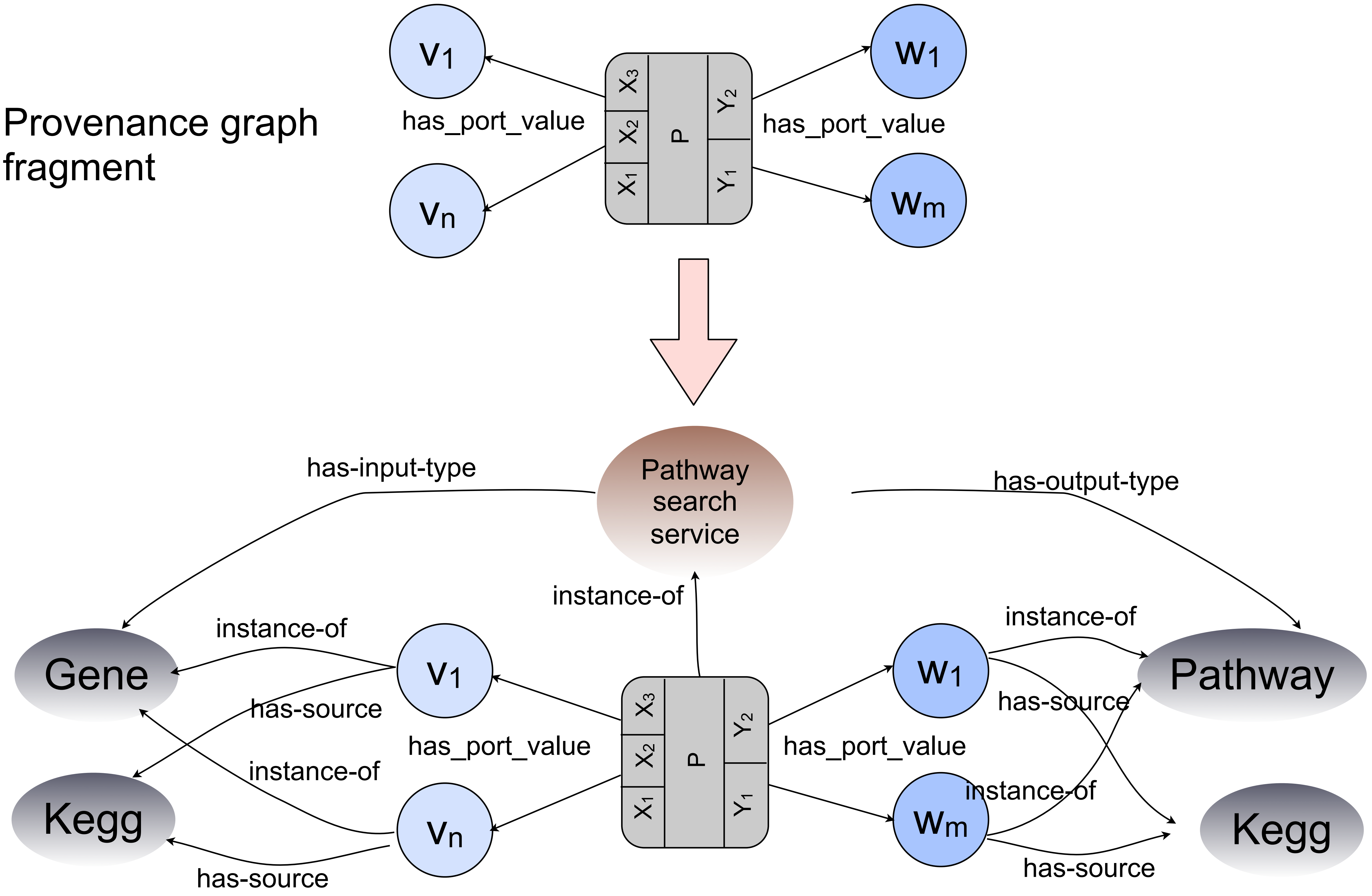


Annotations as semantic overlay

Provenance graph fragment

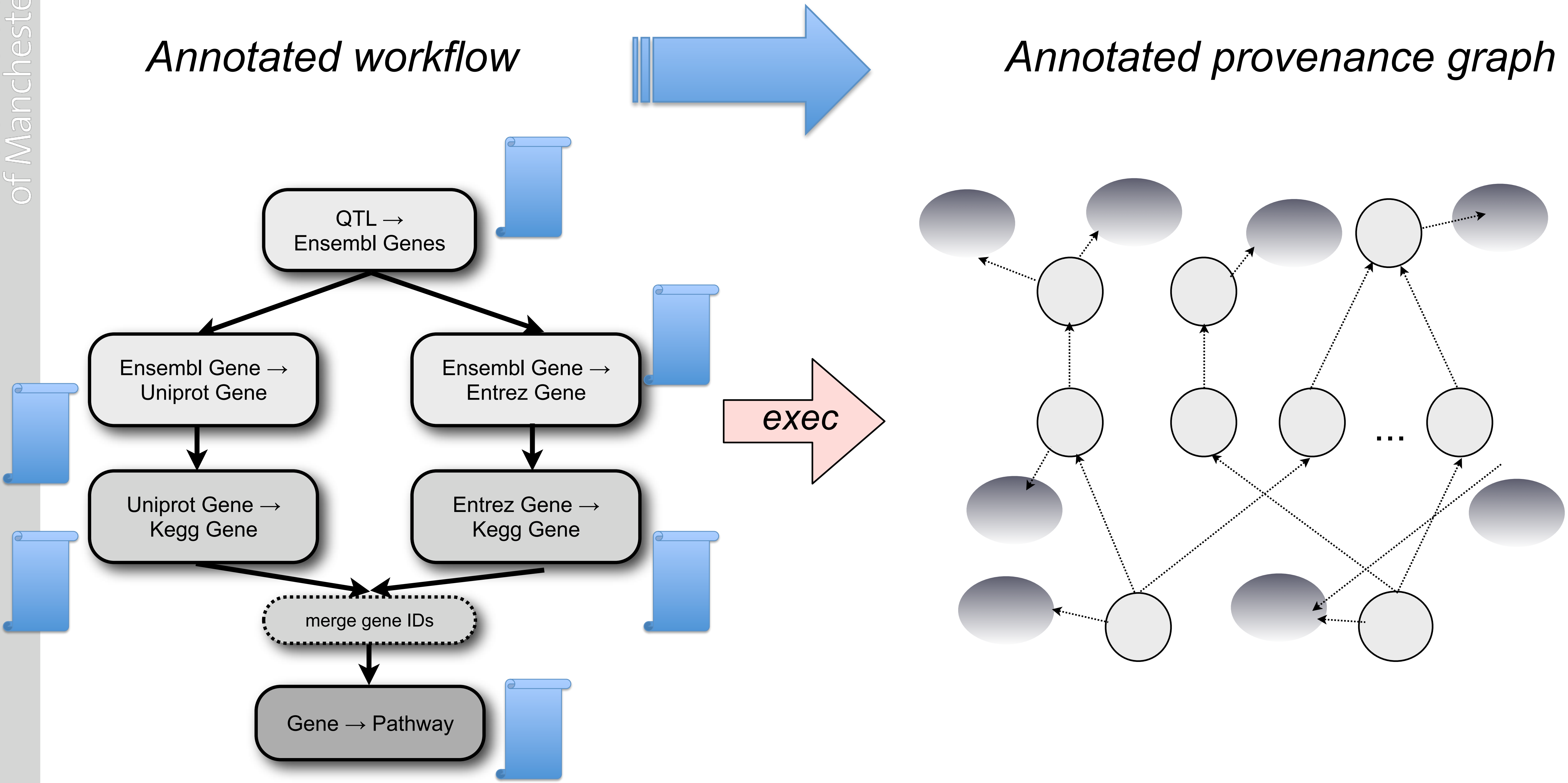


Example Janus domain-aware fragment

```
<rdf:Description rdf:about="http://purl.org/net/taverna/janus/test1625">
<janus:has_iteration>[]</janus:has_iteration>
<rdf:type rdf:resource="http://purl.org/net/taverna/janus#port_value"/>
<rdf:type rdf:resource="http://purl.org/obo/owl/sequence#gene"/>
<janus:has_source rdf:resource="http://purl.org/net/taverna/janus#KEGG"/>
</rdf:Description>
```

this is rule-defined, too

Extensions to Linked Data



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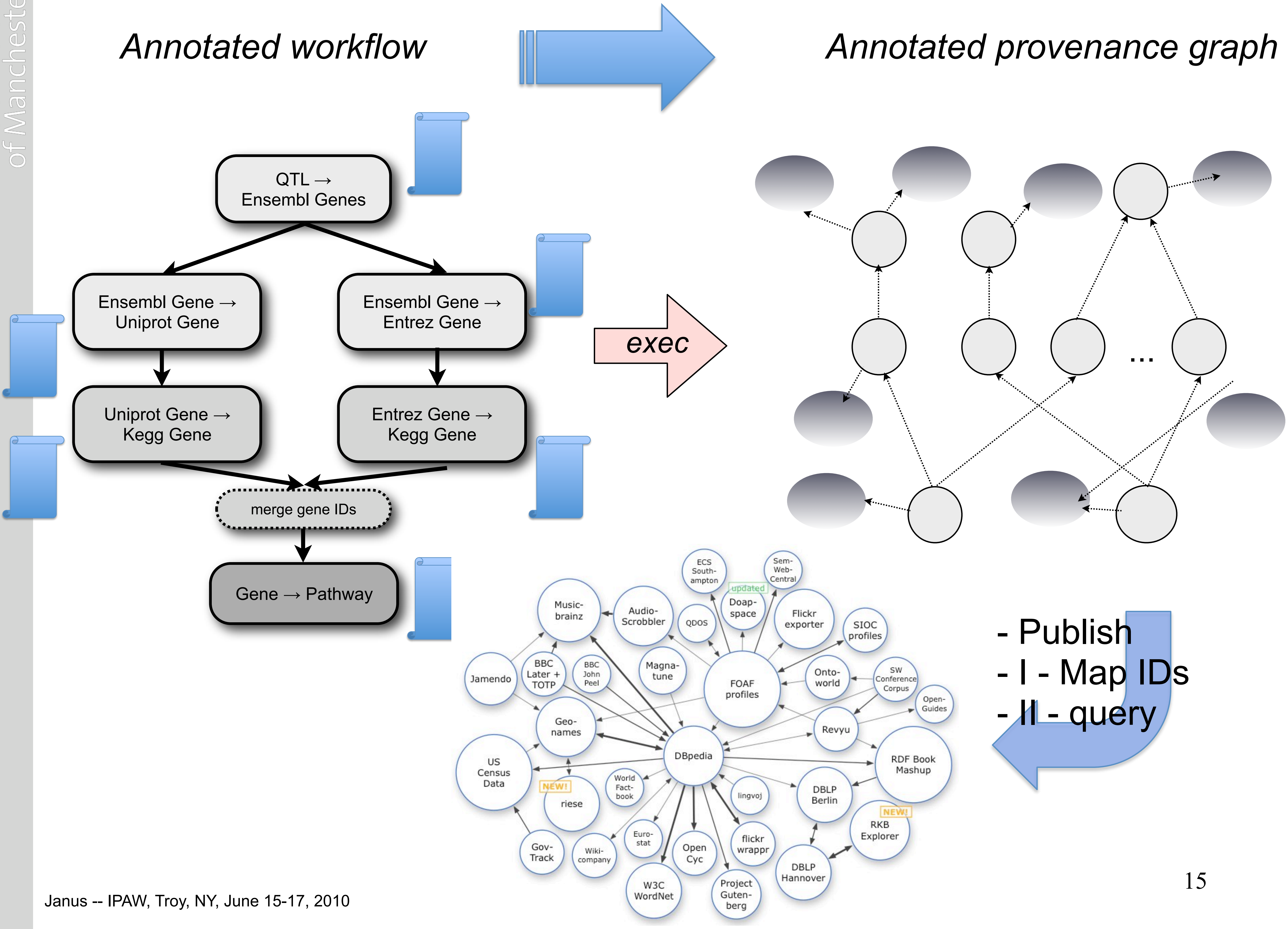
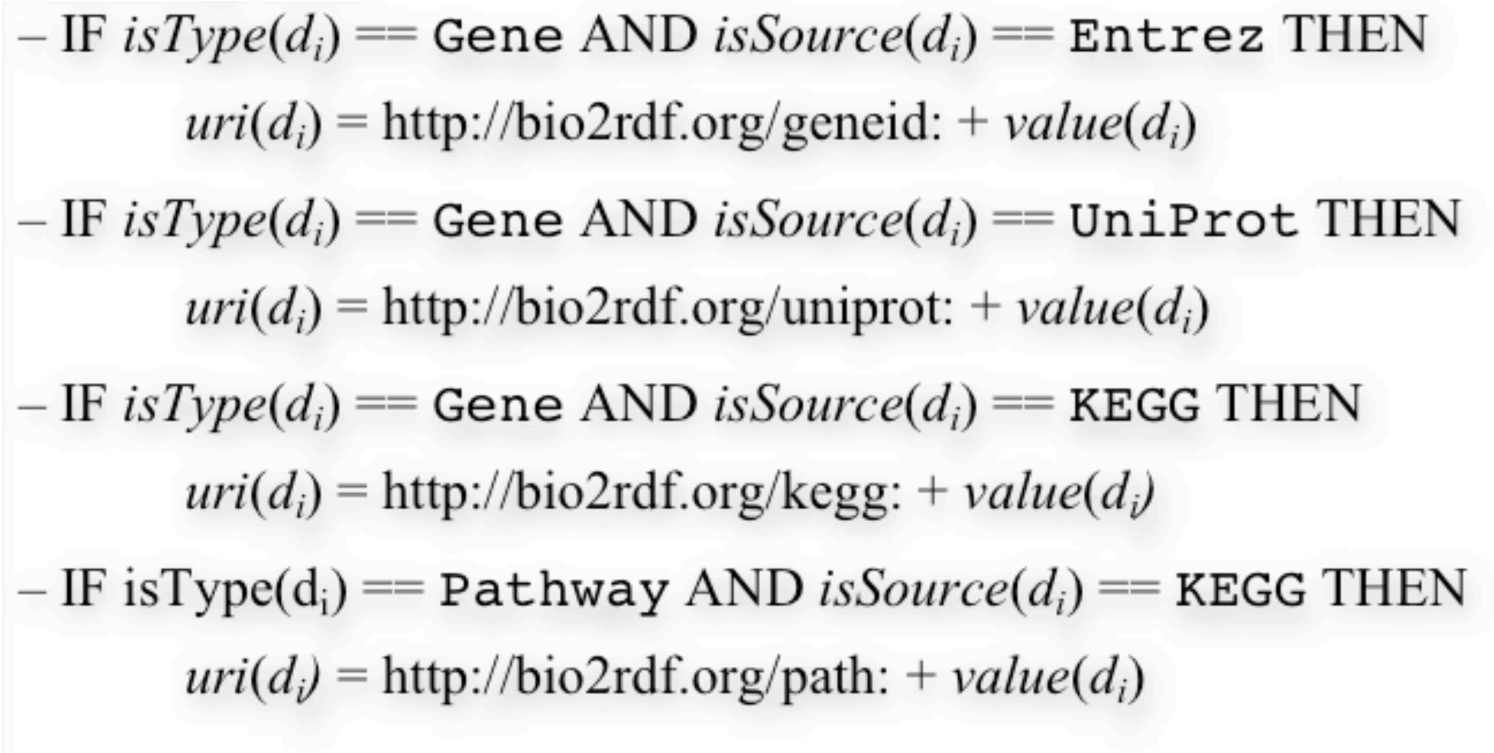


- Publish
- I - Map IDs
- II - query

I - Mapping data values to LoD URIs

In our prototype we map data values to Bio2RDF as follows:



– IF $isType(d_i)$ == Gene AND $isSource(d_i)$ == Entrez THEN

$uri(d_i)$ = http://bio2rdf.org/geneid: + $value(d_i)$

Entrez Genes

– IF $isType(d_i)$ == Gene AND $isSource(d_i)$ == UniProt THEN

$uri(d_i)$ = http://bio2rdf.org/uniprot: + $value(d_i)$

Uniprot Genes

– IF $isType(d_i)$ == Gene AND $isSource(d_i)$ == KEGG THEN

$uri(d_i)$ = http://bio2rdf.org/kegg: + $value(d_i)$

KEGG Genes

– IF isType(d_i) == Pathway AND $isSource(d_i)$ == KEGG THEN

$uri(d_i)$ = http://bio2rdf.org/path: + $value(d_i)$

KEGG Pathways

```
<rdf:Description rdf:about="http://purl.org/net/taverna/janus/create_report/entrezGeneId">
   <janus:has_value_binding rdf:resource="http://purl.org/net/taverna/janus/test18"/>

<rdf:Description rdf:about="http://purl.org/net/taverna/janus/test18">
   <rdf:type rdf:resource="http://purl.org/net/taverna/janus#port_value"/>
   <rdfs:comment>11835</rdfs:comment>
   <rdf:type rdf:resource="http://purl.org/obo/owl/sequence#gene"/>
  <janus:has_source rdf:resource="http://purl.org/net/taverna/janus#entrez_gene"/>

<rdf:Description rdf:about="http://purl.org/net/taverna/janus/test18">
   <rdfs:seeAlso rdf:resource="http://bio2rdf.org/geneid:11835"/>
```

II - extended queries in the LoD setting

Strategy:

- use the SQUIN LoD query engine to query multiple “Web of Data” sources
    - only Bio2RDF in our case
- combine graph patterns on local provenance with conditions on remote LoD graphs

Q5: Find all Entrez genes that encode proteins involved in ATP binding (GO:0005524).

```
PREFIX uniprot: <http://purl.uniprot.org/core/>
PREFIX : <http://www.taverna.org.uk/janus#>
SELECT distinct ?entrezgene
WHERE {
?protein uniprot:classifiedWith <http://bio2rdf.org/go:0005524> .
?entrezgene <http://bio2rdf.org/bio2rdf_resource:xPath> ?protein .
?gene rdfs:seeAlso ?entrezgene
?gene rdf:type :port_gene
?gene :has_source :entrez_gene . }
```

Bio2RDF

local provenance graph

Current status

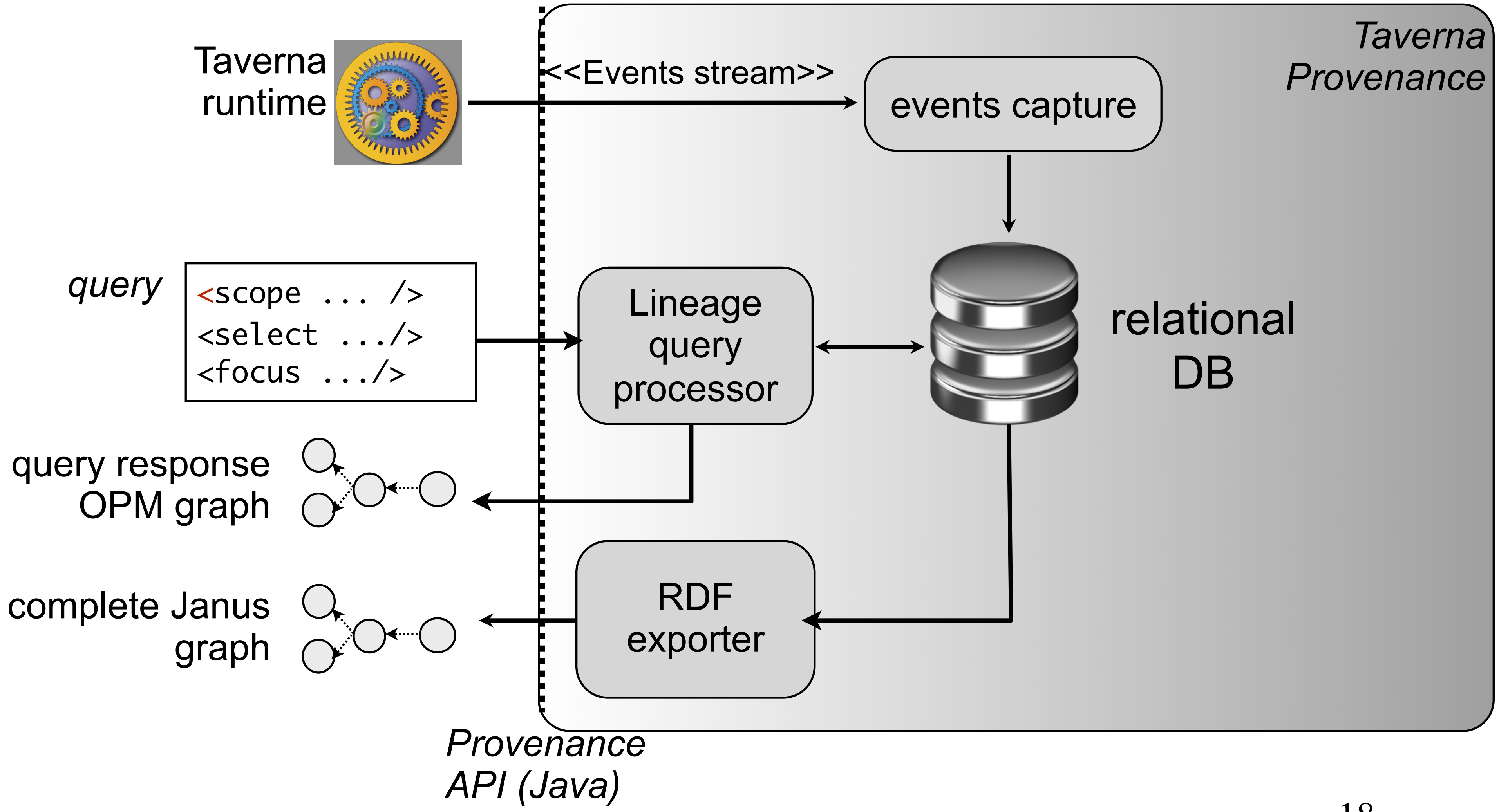
Current Taverna provenance architecture:

Lab prototype

- "Export as..." Janus RDF
- currently only queried using SPARQL
- manually published
- manually annotated

Production

- "native" (relational) graphs
- simple, efficient query language on native provenance



```
<scope ... />
<select .../>
<focus .../>
```

Summary, and moving forward

- Janus: a semantic model for workflow provenance
  - OWL ontology, extension of Provenir
  - should include attribution + system level provenance
  - alignment with OPM?
- Domain-aware graphs through annotations:
  - automatically propagated from workflow annotations when possible
  - but in practice no real workflows are annotated
- LoD integration:
  - powerful provenance publishing and query broadening
  - mapping rules currently limited
  - no completeness guarantee -- all joins are outer joins!