

Semantic Web Technologies

Lecture 11: SWT for the Life Sciences 4: BioRDF and Scientific Workflows

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Outline

BioRDF

- Considerations

- One RDF-ised base

- Toward federation

Scientific workflows

- Introduction

- Scientific workflows in the Semantic Web setting

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- Data integration again (*still...*), but now with new technologies
 - 'bio' having a go at RDF, RDFS, SPARQL and the like
 - Using technologies for newly developed RDFizers, ontology development tools, triplestore tools (e.g., Sesame, Virtuoso, AllegroGraph), and visualisation tools
 - Mesh- vs. mash-ups

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Recollecting the Ruttenberg et al (2007) paper (lecture 8)

- Are (should?) “Tools and strategies to extract or translate from non-RDF data sources to enable their interoperability with data organized as statements.” (be) part of the set of SW Technologies?
 - Or: where are (W3C) standardization efforts for RDBMS→RDF, excel→RDF, OBO→OWL, structured flat file → language y mappings?
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- D2RQ “The mappings allow RDF applications to access the contents of relational databases using Semantic Web query languages like SPARQL. Doing such a mapping requires us to choose how tables, columns, and values in the database map to URIs for classes, properties, instances, and data values.”
 - Name the pros and cons of RDF triplestores vs RDBMSs

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Data integration *strategies* (lecture 8)

- I. Physical schema mappings
 - Global As View (GAV)
 - Local As View (LAV)
 - GLAV
- II. Conceptual model-based data integration
- III. Data federation
- IV. Data warehouses
- V. Data marts
- VI. Services-mediated integration
- VII. Peer-to-peer data integration
- VIII. Ontology-based data integration
 - I or II (possibly in conjunction with the others) through an ontology
 - Linked data by means of an ontology

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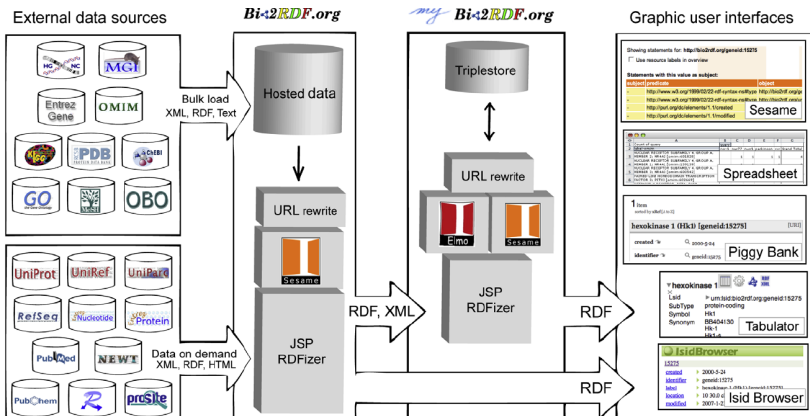
Overview (Bio2RDF as example)

- Data integration with SWT
- What can be achieved with publicly (freely, open source) available tools and data sources
- Main immediate goal of Bio2RDF: convert those data sources to RDF
- How:
 - Bottom-up ontology development of chosen subject domain
 - Decide on architecture: which integration strategy, which data sources, which triplstore, which presentation tools
 - Develop RDF-izer programs (jsp programs HTMLtoRDF, XMLtoRDF, SQLtoRDF, etc)
 - Refinements, a.o.: URI 'normalization': multiple URIs denote the same entity, generate new one, link them with owl:sameAs

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Bio2RDF architecture



from Belleau et al, 2008

First step in the workflow: SeRQL query to fetch basic data from Entrez and GO

```
01  SELECT DISTINCT
02     searchLabel, geneLabel, goLabel
03  FROM
04     {search} rdf:type {<http://bio2rdf.org/bio2rdf#Search>;
05             <http://bio2rdf.org/bio2rdf#query> {searchLabel};
06             rdfs:seeAlso {gene},
07     {gene}   rdfs:label {geneLabel};
08             <http://bio2rdf.org/bio2rdf#xGO> {go},
09     {go}     rdfs:label {goLabel}
```

from Belleau et al, 2008

A consideration

- “An ontology belongs to a community who adapts it, uses it and shares it. With the warehouse stored into a triplestore, it is possible to query the local knowledge base with SeRQL queries. However, the semantic web is meant to be distributed. With more RDF resources available on the web and by using the SPARQL [58] language and protocol, a standard defined by the W3C, the data warehousing concept could become obsolete in the future. This is one perspective of the semantic web.”

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One strategy for a “virtual repository”, various architectures and tools¹

- OWL mappings to provide an integrated list of receptors and executes individual queries against different SPARQL endpoints (receptor explorer)
- AIDA Toolkit for cooperatively search, annotate, interpret, and enrich large collections of heterogeneous documents from diverse locations
- FeDeRate enables a global SPARQL query to be decomposed into subqueries against the remote databases offering either SPARQL or SQL query interfaces.
- Vocabulary of interlinked Datasets (voiD) to create metadata for describing datasets exposed as Linked Data URIs or SPARQL endpoints

¹Kei-Hoi Cheung, H Robert Frost, M Scott Marshall, Eric Prudhommeaux, Matthias Samwald, Jun Zhao, and Adrian Paschke. A journey to Semantic Web query federation in the life sciences. *BMC Bioinformatics* 2009, 10(Suppl 10):S10

Differences

- The layer at which the virtual repository abstraction is supported:
 - Receptor Explorer: Semantic Service Bus (ESB + Jena + Sesame) API exposed to client applications
 - AIDA toolkit: web services, using the SOA API exposed to client applications by WSDL
 - FeDeRate: at the SPARQL query interface
- Generality of approach:
 - Receptor Explorer is a single scenario with step-wise exploration/navigation
 - AIDA Search interface is general-purpose and can be utilized to explore a wide range of RDF data retrieved from multiple locations (SKOS + Sesame, Virtuoso)
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FeDeRate's approach to query management

- Use the common variables in a SPARQL query to decompose it into separate queries for the different data sources; e.g., connecting them by a common human EntrezGene identifier:

```
SELECT ?iupharNm ?type ?label
...
GRAPH <source1> {
  ?iuphar iface:iupharName ?iupharNm .
  ?human iface:iuphar ?iuphar .
  ?human iface:geneName ``GABBR1'' .
  ?human iface:entrezGene ?humanEntrez }
GRAPH <source2> {
  ?gene db:entrezgene ?humanEntrez ;
  ?gene a ?type ;
  ?gene rdfs:label ?label }
```

FeDeRate's approach to query management

- Determines which variables in each GRAPH constraint are present in the SELECT (or are referenced in subsequent graph patterns), then translate the constraint into a subordinate SPARQL query:

```
SELECT ?iupharNm ?humanEntrez
FROM <source1>
WHERE {
    ?iuphar iface:iupharName ?iupharNm .
    ?human iface:iuphar ?iuphar .
    ?human iface:geneName ``GABBR1`` .
    ?human iface:entrezGene ?humanEntrez }
```

FeDeRate's approach to query management

- Subsequent subordinate queries with bindings constraining the variables bound by earlier queries, expressed as standard SPARQL constraints:

```
FROM <source2>  
WHERE {  
  ?gene db:entrezgene ?humanEntrez ;  
  ?gene a ?type ;  
  ?gene rdfs:label ?label  
FILTER (?humanEntrez = 2550 ||  
        ?humanEntrez = 9568)}
```

Consideration

- The billion triple challenge
- Focus on data or on knowledge; how to combine it?
- Scalability
- Date integration strategy

Some recent observations from LODD

- A significant challenge ... is the strong prevalence of terminology conflicts, synonyms, and homonyms. These problems are not addressed by simply making data sets available on the Web using RDF as common syntax but require deeper semantic integration
- For applications that focus on discovery and data navigation, having explicit links between data sources is often already a huge benefit even without semantic integration
- **For other applications that rely on expressive querying or automated reasoning deeper integration is essential ...**, it would be beneficial if more community practices on publishing term and schema mappings would be established

Anja Jentsch, Bo Andersson, Oktie Hassanzadeh, Susie Stephens, Christian Bizer. Enabling Tailored Therapeutics with Linked Data. LDOW2009, April 20, 2009, Madrid, Spain.

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Requirements²

- Seamless access to resources and service
- Service composition & reuse and workflow design
- Scalability
- Detached execution
- Reliability and fault-tolerance
- User-interaction
- “Smart” re-runs
- “Smart” (semantic) links
- Data provenance

²Ludäscher et al. Scientific Workflow Management and the Kepler System.

Some general characteristics of Scientific Workflows³

- The ability to handle many and varied analysis tools; not merely database systems that have to be linked up, but the many (custom-made) analysis tools w.r.t. amount of databases
- Interfaces to a diverse range of computational environments (supercomputers, grid, Internet and Semantic Web)
- The ability to handle activity mixes that are different from typical business profiles—and there are, at least initially, few canned and reusable workflows (i.e., design from scratch)
- Need for explicit representation of knowledge at different stages
- Auditability of the computations (when the results are used to make decisions that carry regulatory or legislative implications; e.g., data analysis of clinical trials, climate model predictions)

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Further additions w.r.t. bio and the Semantic Web

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- Repeatability of the *in silico* experiment
- Customization of the data sources and methods for each researcher
- ‘open’ system
- Provenance of the data; or: a need for addressing the **trust** layer in the Semantic Web layer cake

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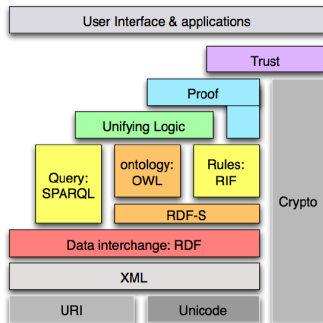
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Where can we plug SWT languages into Scientific Workflows?

- **RDF: common data format (for linking and integration)**
- SPARQL: querying data
- OWL: representation of the knowledge across the workflow
- Rules: orchestrate the service execution
- Services (e.g., WSDL, OWL-S): to discover useful scripts that can perform a task in the workflow
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Examples w.r.t. SWT

- Taverna, on top of *my*Grid
 - RDF for data interoperability, for provenance
 - RDF query language for querying the RDF data
 - OWL ontologies for the domain, for the services, for the workflows; for consistency checking, taxonomic classification
 - WSMO's tasks
 - Jena, Sesame, Protégé
- Kepler, on top of Ptolemy
 - services
 - explorations with ontologies
- Wings, on top of Pegasus
 - ontologies (OWL), reasoning (with Jena)

Provenance and trust, system examples

- Taverna: experiment-, workflow-, and knowledge-provenance, representing a mixture of RDF(S) and OWL to represent the overall model, individual provenance graphs of a particular workflow⁴
- PASS experiments, with another provenance ontology for the workflow⁵, and Pychinko, a Semantic Web rule engine to orchestrate the service execution⁶

⁴ Carole Goble et al. Knowledge Discovery for biology with Taverna. In: *Semantic Web: Revolutionizing knowledge discovery in the life sciences*. 2007, pp355-395.

⁵ <http://provenance.mindswap.org/provenance.owl>

⁶ Jennifer Golbeck and James Hendler. A Semantic Web Approach to the Provenance Challenge. *Concurrency Computat.: Pract. Exper.*, 2007

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