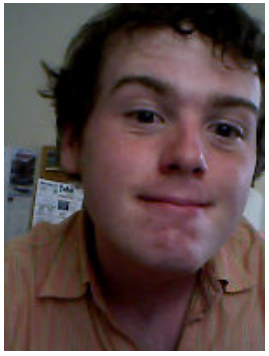
Extension of Galaxy to Utilize Web Services and A Semantic Suggestion Engine

Alok Dhamanaskar, Akshay Choche, Michael E. Cotterell, Jie Zheng, Christian Stoeckert Jr., Jessica C. Kissinger and John A. Miller

University of Georgia and University of Pennsylvania, USA

Alok Dhamanaskar

Akshay Choche



Michael Cotterell

Chris Stoeckert

John Miller

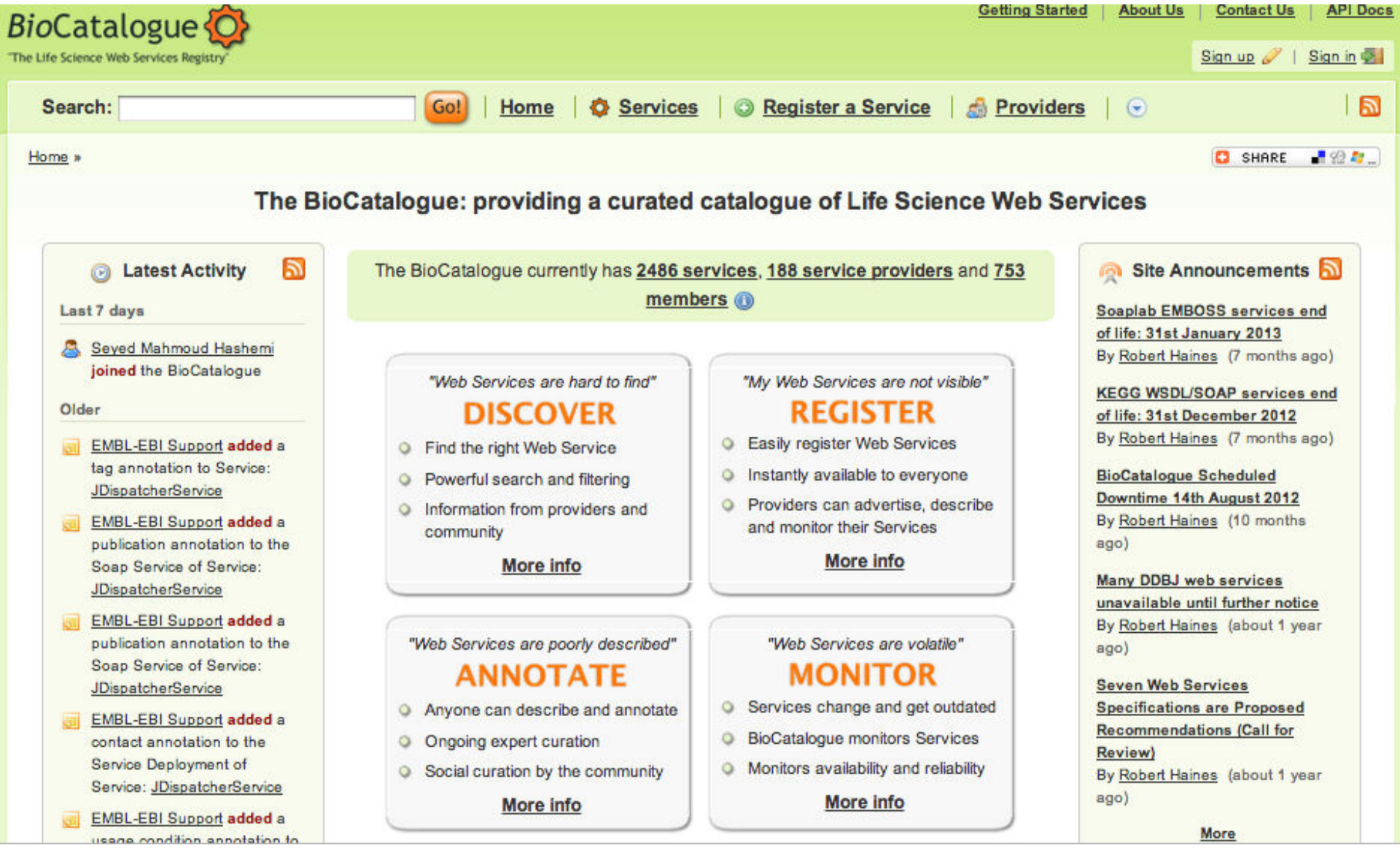
The Motivation:

Galaxy is currently restricted to tools/data resources that are wrapped specifically for Galaxy and manually added either via and tool wrapper and addition to tools_conf.xml or addition via the tool shed.

Wouldn't it be nice if Galaxy could utilize any tool that is publicly exposed via a Web service with just a click?

What are Web services?

- A web service is any piece of software that makes itself available over the internet and uses a standardized XML messaging system. XML is used to encode all communications to a web service. For example, a client invokes a web service by sending an XML message, then waits for a corresponding XML response. Because all communication is in XML, web services are not tied to any one operating system or programming language--Java can talk with Perl; Windows applications can talk with Unix applications.
- Web services come in two flavors:
  - SOAP services described by WSDL XML documents
  - RESTful services described by WADL XML documents



http://www.biocatalogue.org

Enabling Galaxy to Invoke Web services

Prerequisites:

- SSH/Terminal Access to Galaxy Installation
- Java 7 SE or EE (Oracle or OpenJDK)
- Python 2.6+
- JPype Python Library

Enabling Galaxy to Invoke Web services

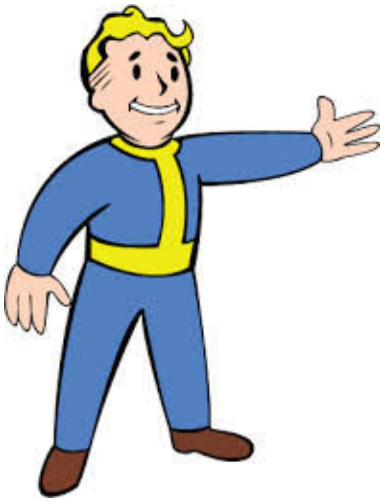
Installation is Easy!

1. Set Environment Variables

```
galaxy@galaxy:~/galaxy-dist$ export JAVA_HOME=/usr/lib/jvm/java-7-openjdk-amd64
galaxy@galaxy:~/galaxy-dist$ export GALAXY_HOME=$(pwd)
galaxy@galaxy:~/galaxy-dist$
```

Enabling Galaxy to Invoke Web services

Installation is Easy!



1. Set Environment Variables → 2. Download Installation Script

```
galaxy@galaxy:~/galaxy-dist$ cd
galaxy@galaxy:~$ wget http://mango.ctegd.uga.edu/jkissingLab/SWS/Galaxy
--2013-06-21 12:06:16--  http://mango.ctegd.uga.edu/jkissingLab/SWS/Gal
Resolving mango.ctegd.uga.edu (mango.ctegd.uga.edu)... 128.192.99.13
Connecting to mango.ctegd.uga.edu (mango.ctegd.uga.edu)|128.192.99.13|:
HTTP request sent, awaiting response... 200 OK
Length: 41656528 (40M) [application/zip]
Saving to: `WSExtensionTool.zip'

100%[==========================================================================

2013-06-21 12:06:17 (111 MB/s) - `WSExtensionTool.zip' saved [41656528/

galaxy@galaxy:~$ unzip WSExtensionTool.zip
```

Enabling Galaxy to Invoke Web services

Installation is Easy!

1. Set Environment Variables → 2. Download Installation Script → 3. Run Installation Script

```
galaxy@galaxy:~$ cd WS\ Extension\ Tool/
galaxy@galaxy:~/WS Extension Tool$ python install.py
Preparing to install the new WS Extension tool
Copied the folder 'WebServiceToolWorkflow_REST_SOAP' to /home/galaxy/ga
The "Add Web Service Tool" added successfully
The "Web Service Tools" added successfully
The section "Web Service Workflow Tools" is added successfully
Workflow disabling Code added to __init__.py
Refresh Code added to __init__.py
Refresh code is added to app.py
****Installation of tool is complete. Now reload galaxy to use the inst
galaxy@galaxy:~/WS Extension Tool$
```

Enabling Galaxy to Invoke Web services

Installation is Easy!

1. Set Environment Variables → 2. Download Installation Script → 3. Run Installation Script

Now the Web Service tool has been installed and added to Galaxy's tool_conf.xml file.

tool_conf.xml → Web Service Tool

However, you need to

Restart Galaxy

for tool_conf.xml changes to take effect!

Enabling Galaxy to Invoke Web services

Installation is Easy!

1. Set Enviro… Va…
2. Download Installati… Scr…
3. Run Installation Script

…ool
ha… …added
…file.

tool_conf.xml

WEB SERVICE TOOLS

Add Web service tool(s)

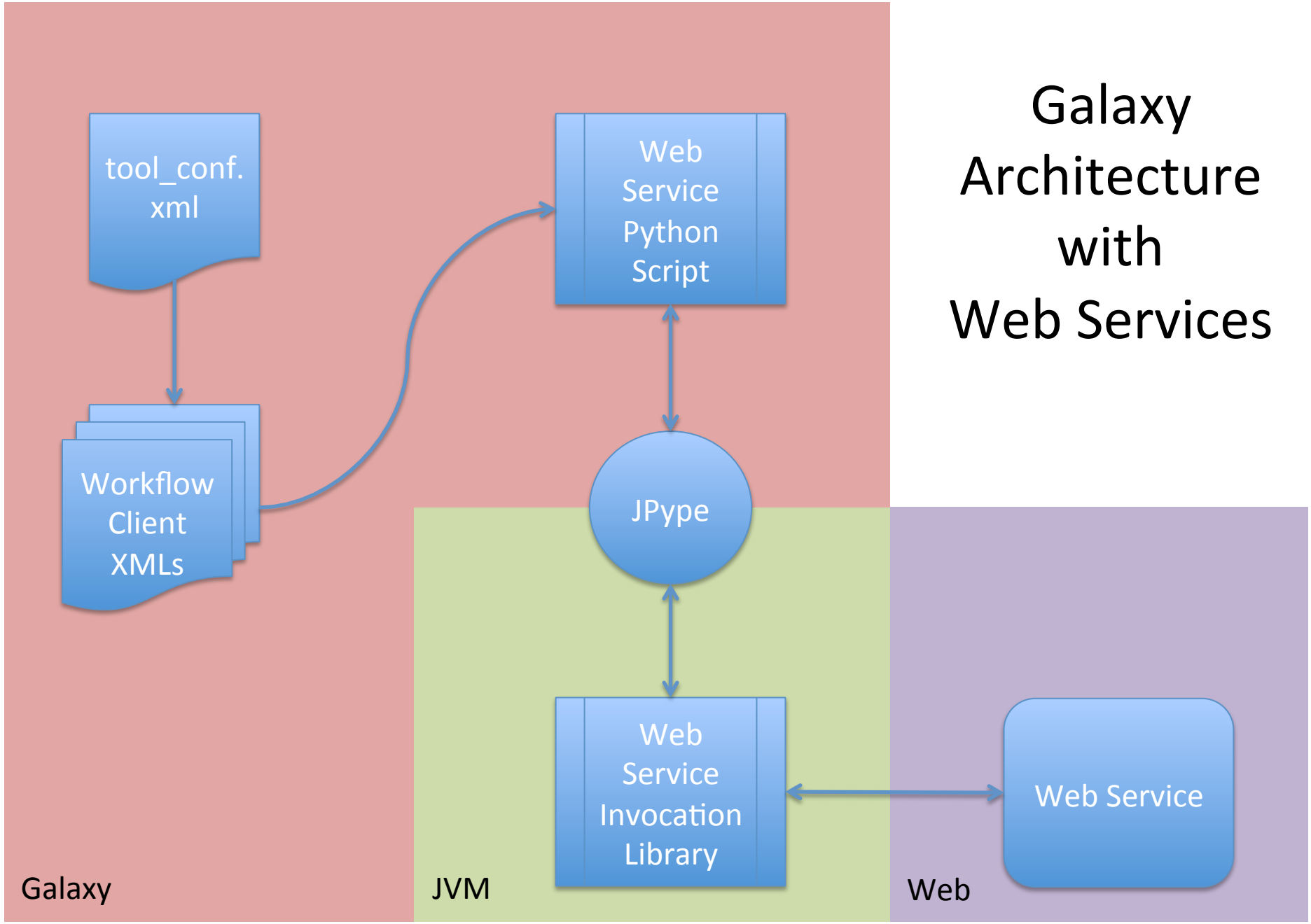
- Step a: Enter the URL (WSDL/WADL location) of tool (web service) description document
- Step b: Select desired Web Service Tools / Operations to be added.
- Step c: Add tool(s) to Galaxy

However, you ne…d to

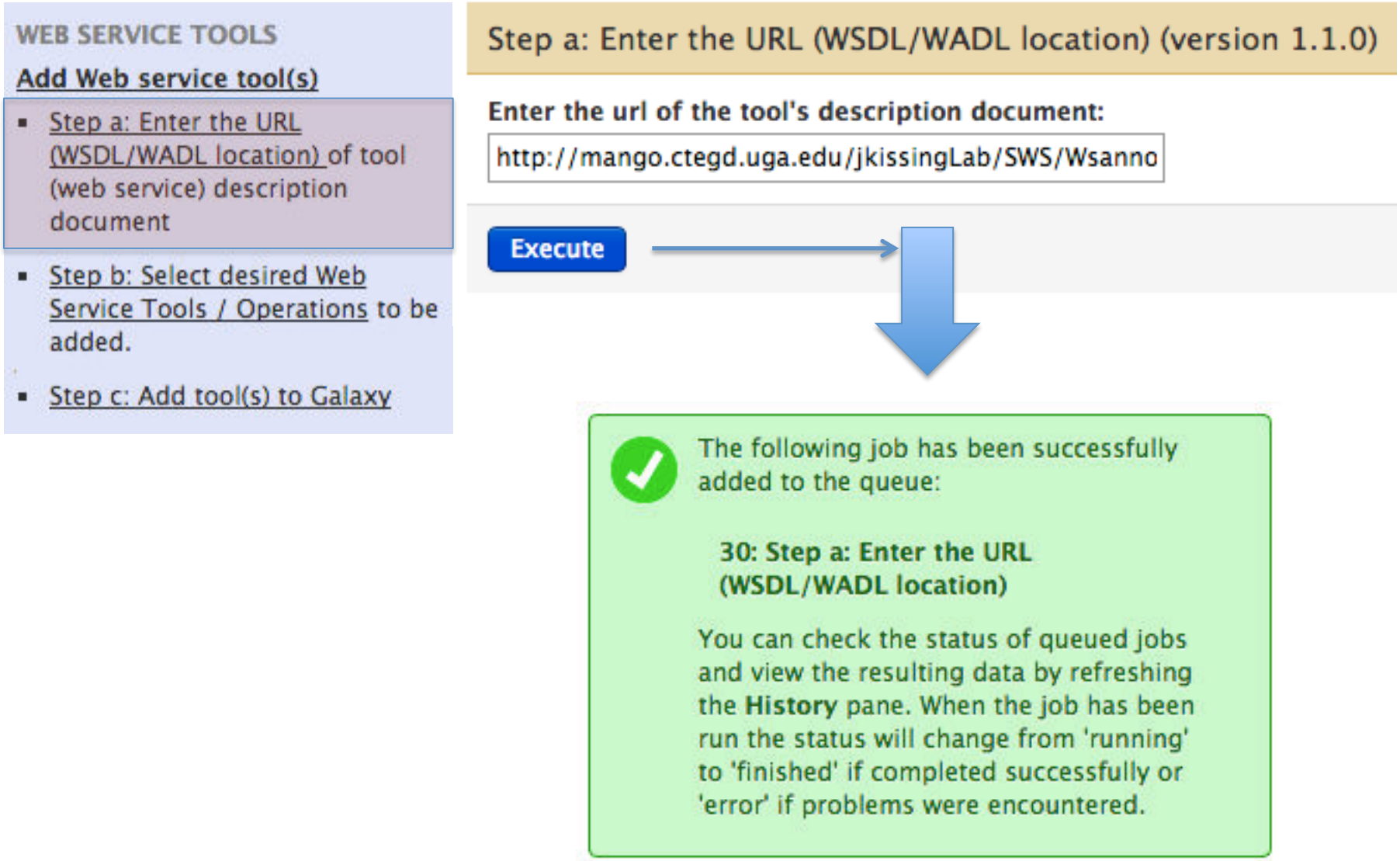
Restart Galaxy

for tool_conf.xml changes to take effect!

Web Service Tool


Galaxy Architecture with Web Services
tool_conf. xml
Web Service Python Script
Workflow Client XMLs
JPype
Web Service Invocation Library
Web Service
Galaxy
JVM
Web

Using Web Services in Galaxy

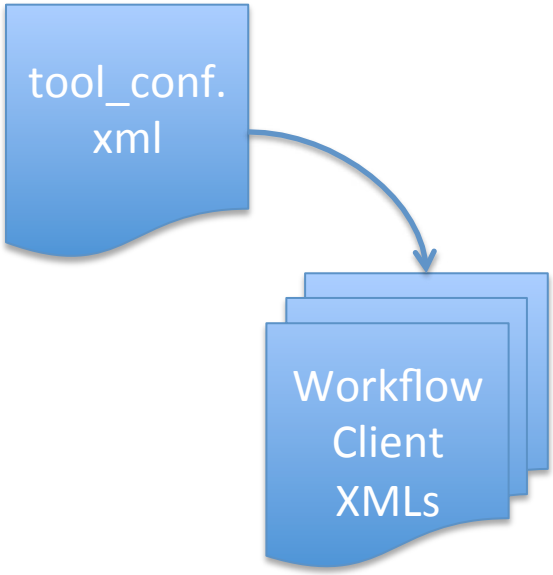


Using Web Services in Galaxy

WEB SERVICE TOOLS

Add Web service tool(s)

- Step a: Enter the URL (WSDL/WADL location) of tool (web service) description document
- Step b: Select desired Web Service Tools / Operations to be added.
- Step c: Add tool(s) to Galaxy



Step b: Select desired Web Service Tools / Operations (version 1.1.0)

1. The previous step was (No action required) :

30: Step a: Enter the.. location)

You can also select any previously performed Step a from the history to avoid repeated execution of Step a.

2. The tool specified by the Web service is:

http://mango.ctegd.uga.edu/jkissingLab/SWS/Wsannotation/resources/clustalv

Displays the tool (Web service) chosen in Step a. No action required.

3. Select functions of the Web service tool to add to galaxy:

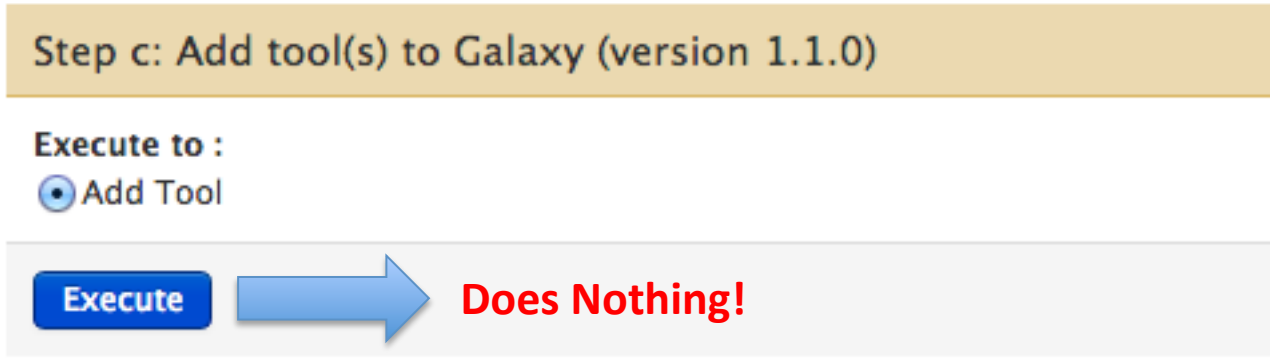
Select All | Unselect All

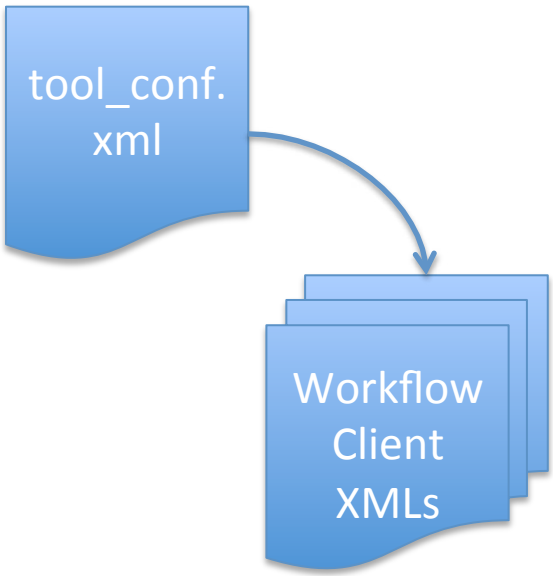
- run
- getStatus
- getResultTypes
- getResult
- getParameters
- getParameterDetails

Some tools have more than one function. It is important to select the appropriate functions.

Execute → **Generates Workflow Client XML Files**

Using Web Services in Galaxy



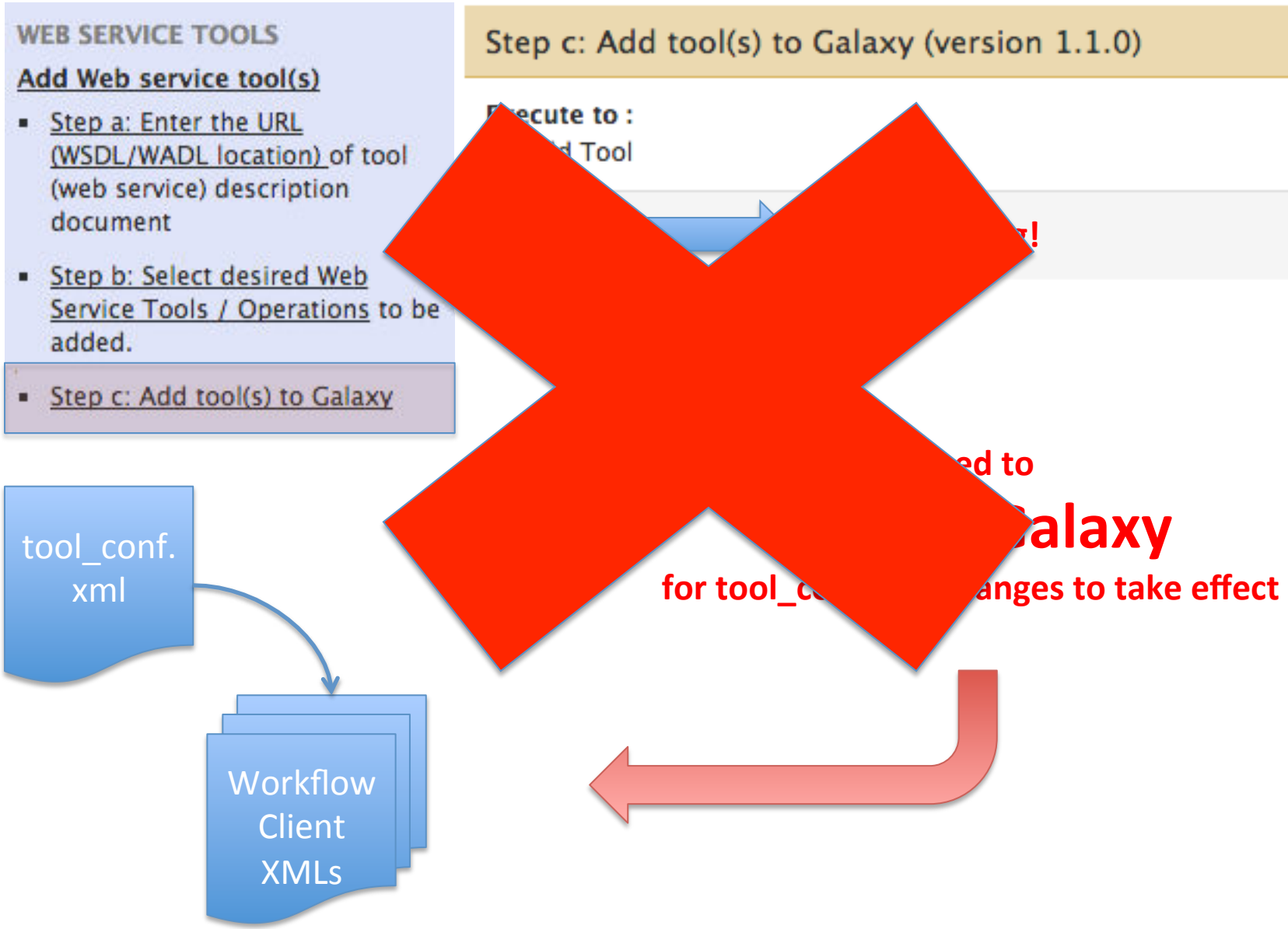


Need to

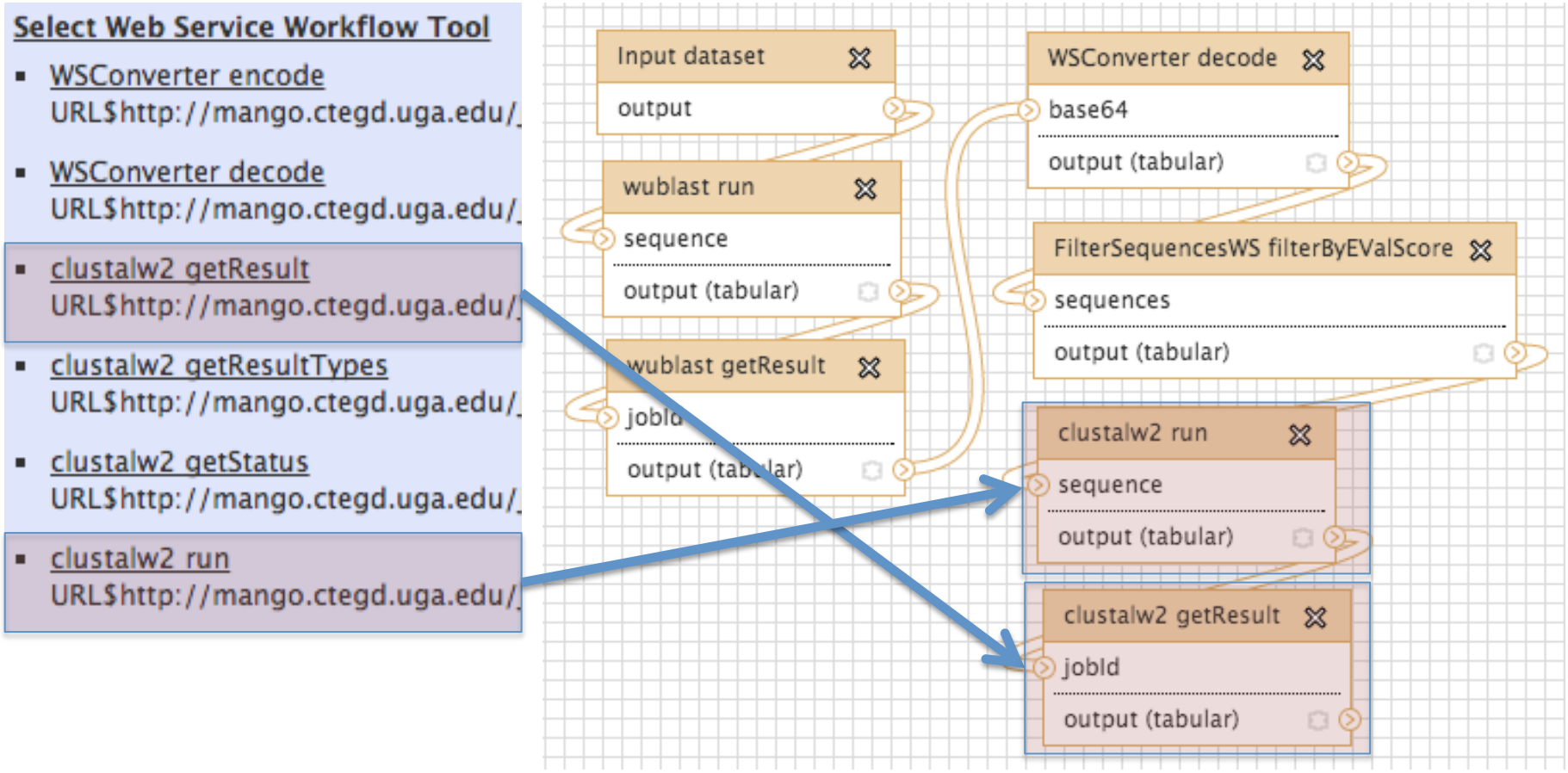
Restart Galaxy

for tool_conf.xml changes to take effect

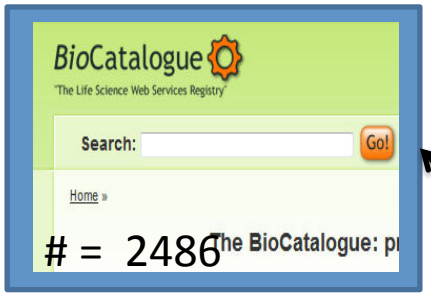
Using Web Services in Galaxy

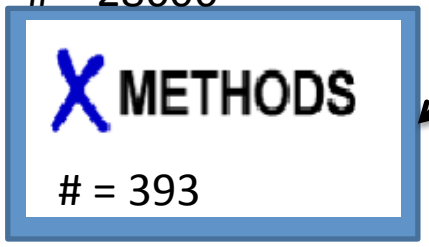


Web Services can be used in Workflows



Find Services / Tools for My Workflow





#354

#93

#0

#36

Seems like a lot of services to look through ! I wonder if I missed any ?

Sequence Alignment Search

Total Services = 483 with maybe 1000s of operations

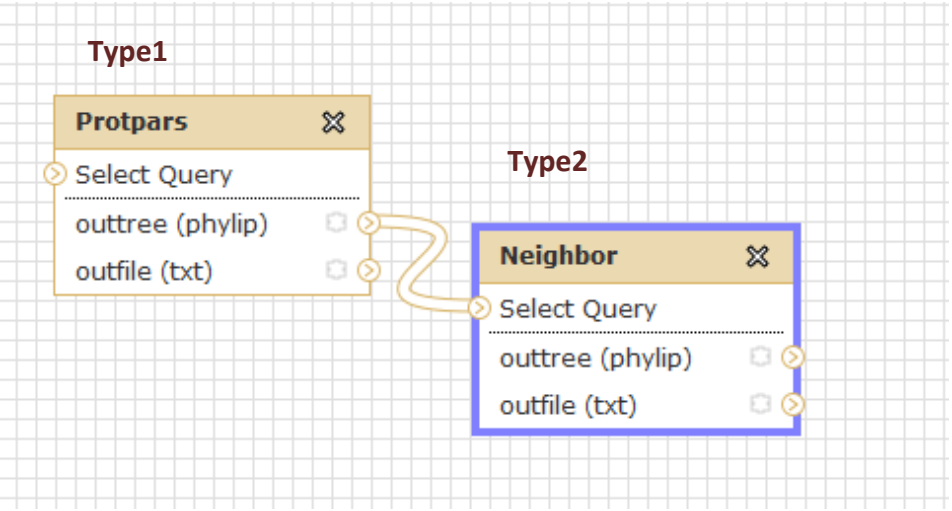
Popular Web service Registries

Tools available in Galaxy + Tools in the Galaxy Tool-shed

Service Discovery

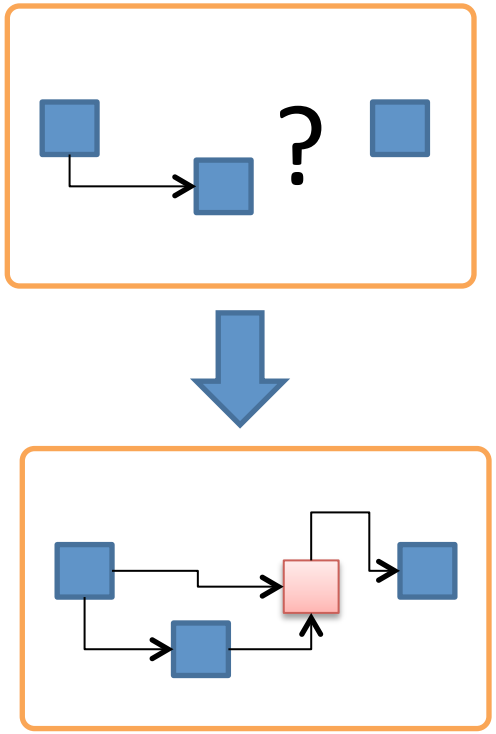
Find Input-Output Compatible Services

I selected 2 of those operations, entered them in my workflow designer, but when I tested, it didn't work.



Input output Matching Problem

Connect the Newly Added Service into the Workflow



Wish I could figure out which service operation(s) might fill the gap in my workflow.

Why can't the software make a suggestion?

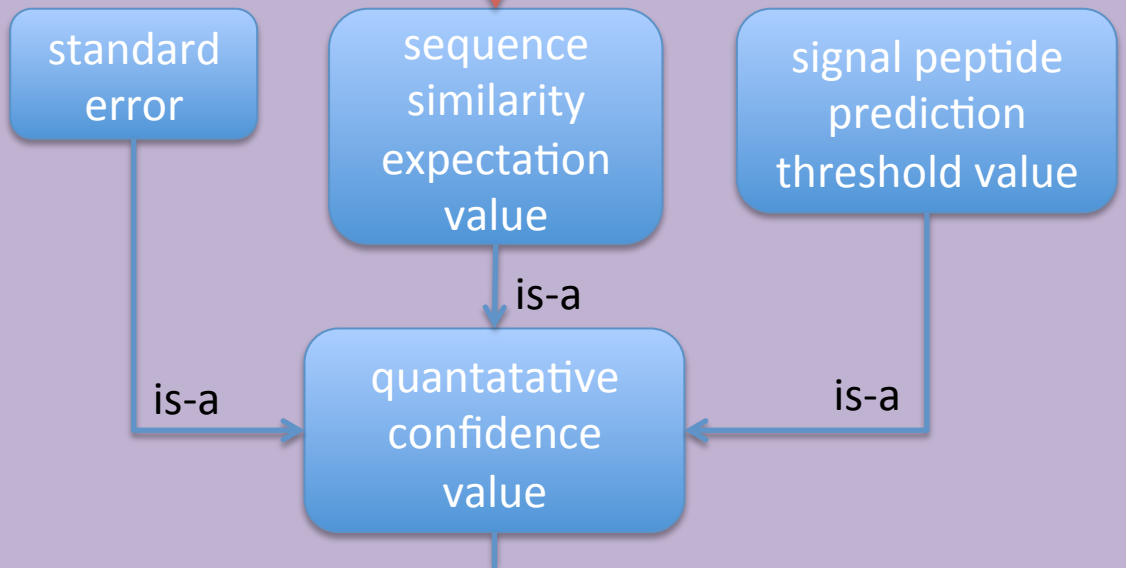
Workflow design / service composition

Semantically Annotated Web Services

wublast.sawsdl – Semantically Annotated WSDL for WU-BLAST

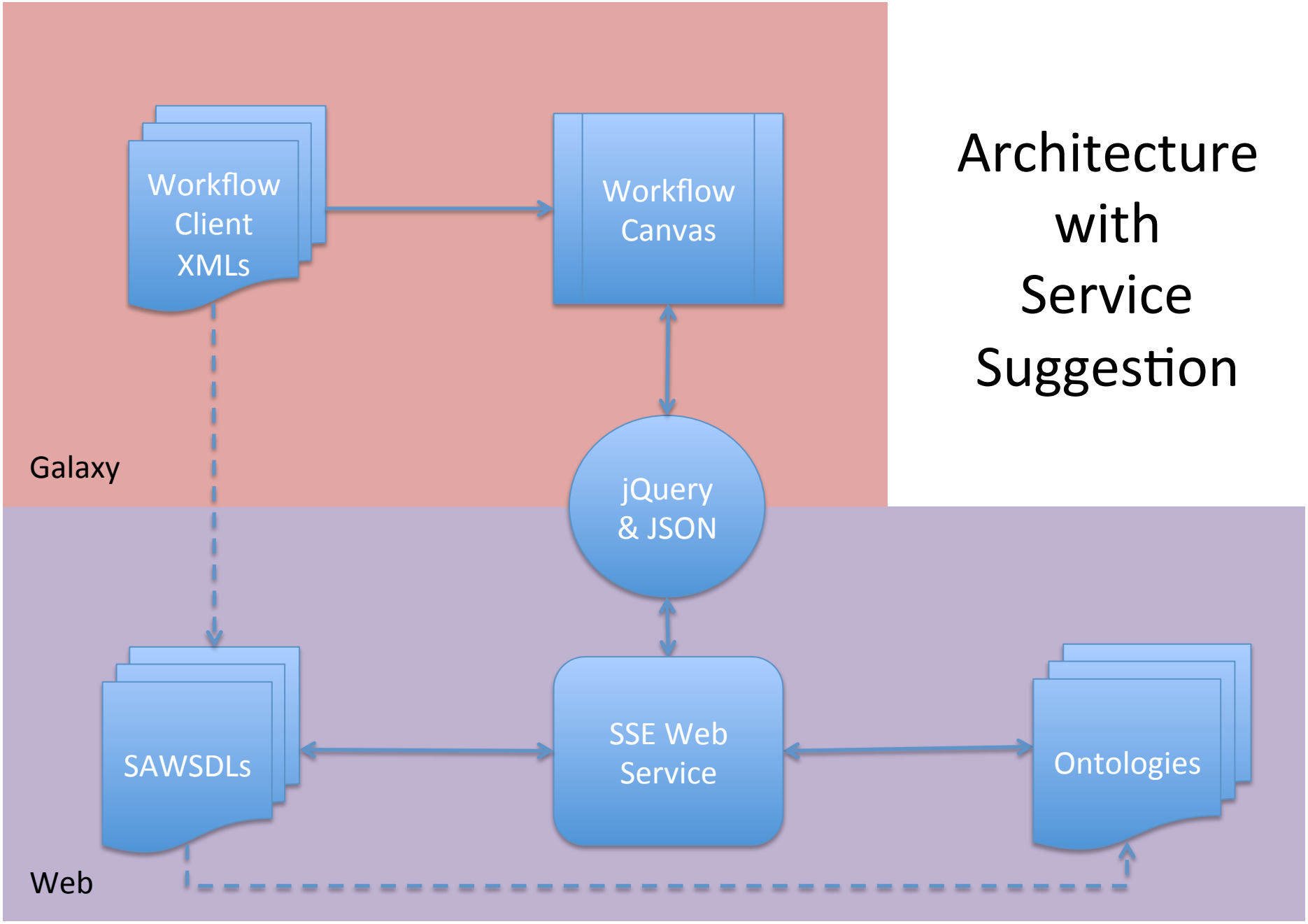
```
▼<xsd:element minOccurs="0" maxOccurs="1" name="exp" nillable="true" type="xsd:string"
 sawsdl:modelReference="http://purl.obolibrary.org/obo/OBIws_0000082">
  ▼<xsd:annotation>
    ▼<xsd:documentation xml:lang="en">
       Expectation value threshold [Limits the number of scores and alignments reported
       times the match is expected to occur by chance.]
     </xsd:documentation>
   </xsd:annotation>
 </xsd:element>
```

http://purl.obolibrary.org/obo/OBIws_0000082

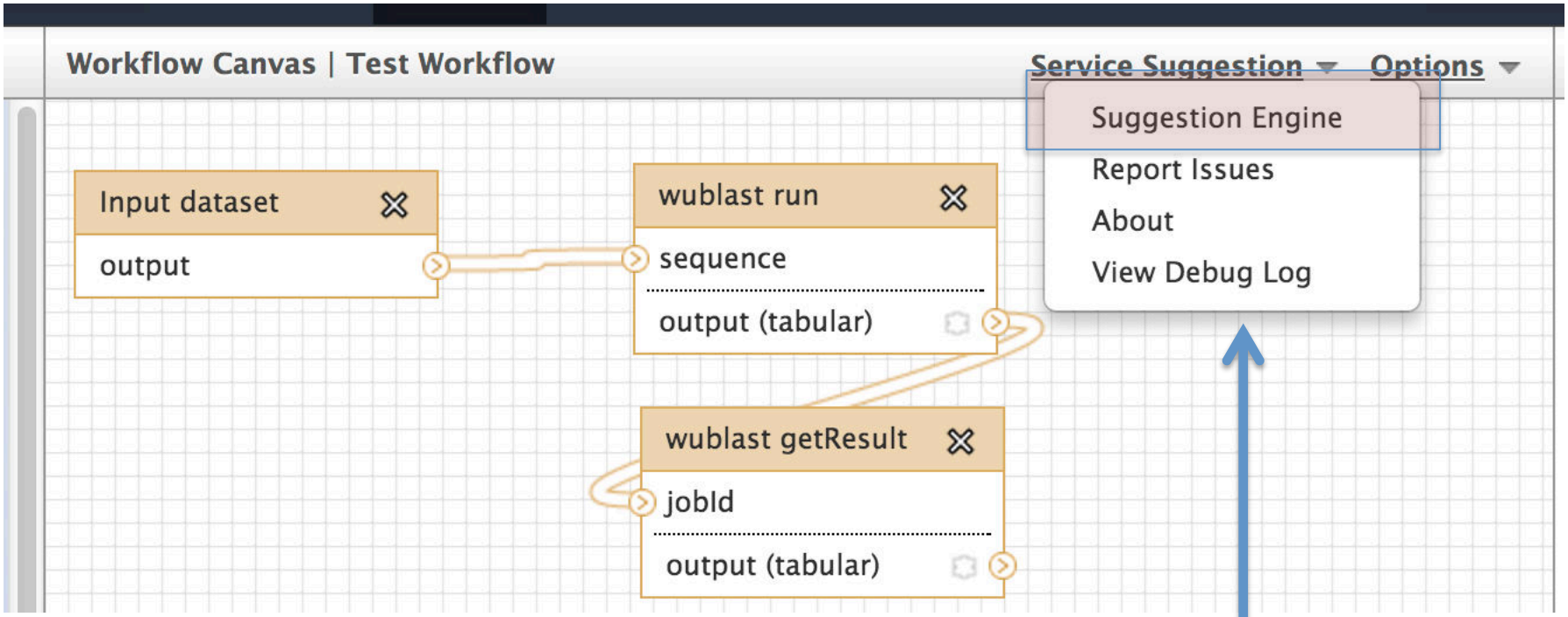


Ontology – OBIws

Architecture with Service Suggestion



Service Suggestion



Modified the UI using minimal mako modifications and some jQuery magic!

Service Suggestion

1. Choose the type of suggestion you want

Forward Suggestion

Backward Suggestion

Bidirectional Suggestion

Details

Service Suggestion Engine

Version: 1.6

[-] Setup & Run Query

Choose Suggestion Type:

Choose the kind of suggestions you want by indicating where you think they should go in the workflow.

Forward Suggestion

Click here for more information about the different types of service suggestion.

Tools to Feed From:

Select the tools in current workflow that you think should feed into suggested service operations.

Step 2 – wublast getResult

Step 2 – wublast getResult

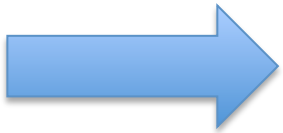
Goal / Purpose:

In simple terms, describe what you are trying to do/find (e.g., multiple

Service Suggestion

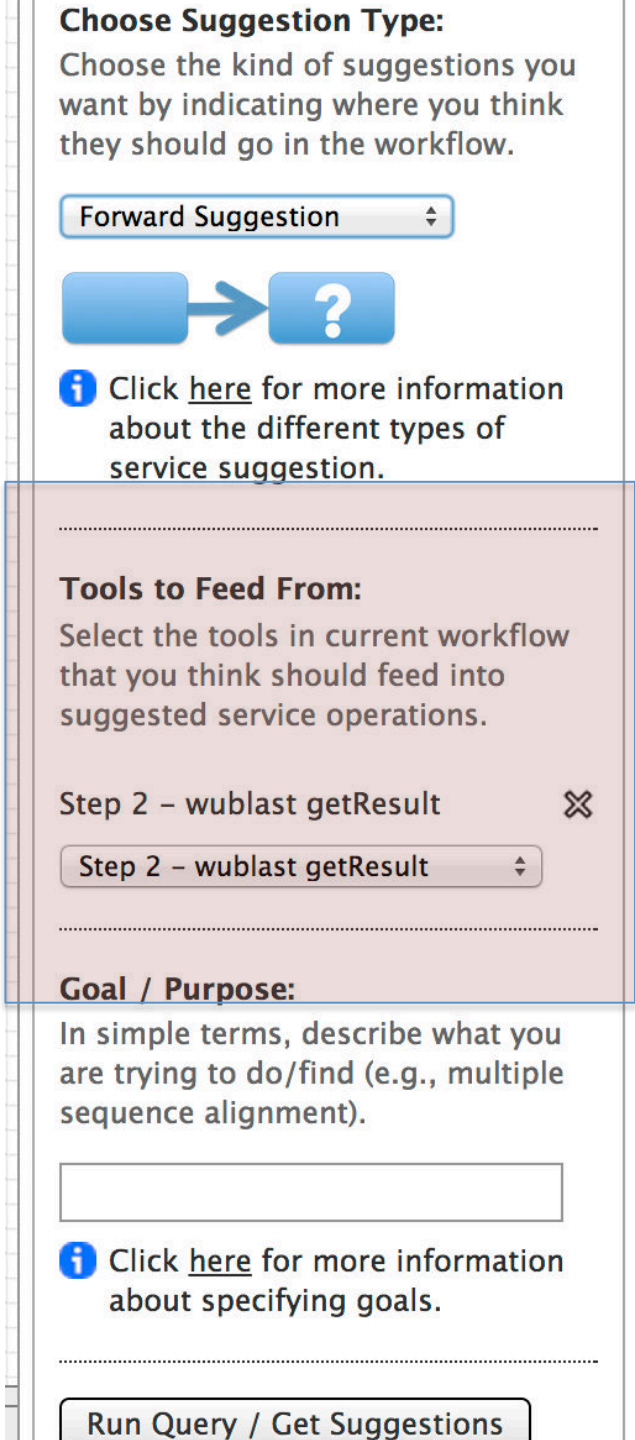
1. Choose the type of suggestion you want

2. Select Relevant Tools



The tools currently on the canvas will appear in one ore more dropdown lists (depending on suggestion type).

Select specific ones to utilize for suggestion or choose “all”.

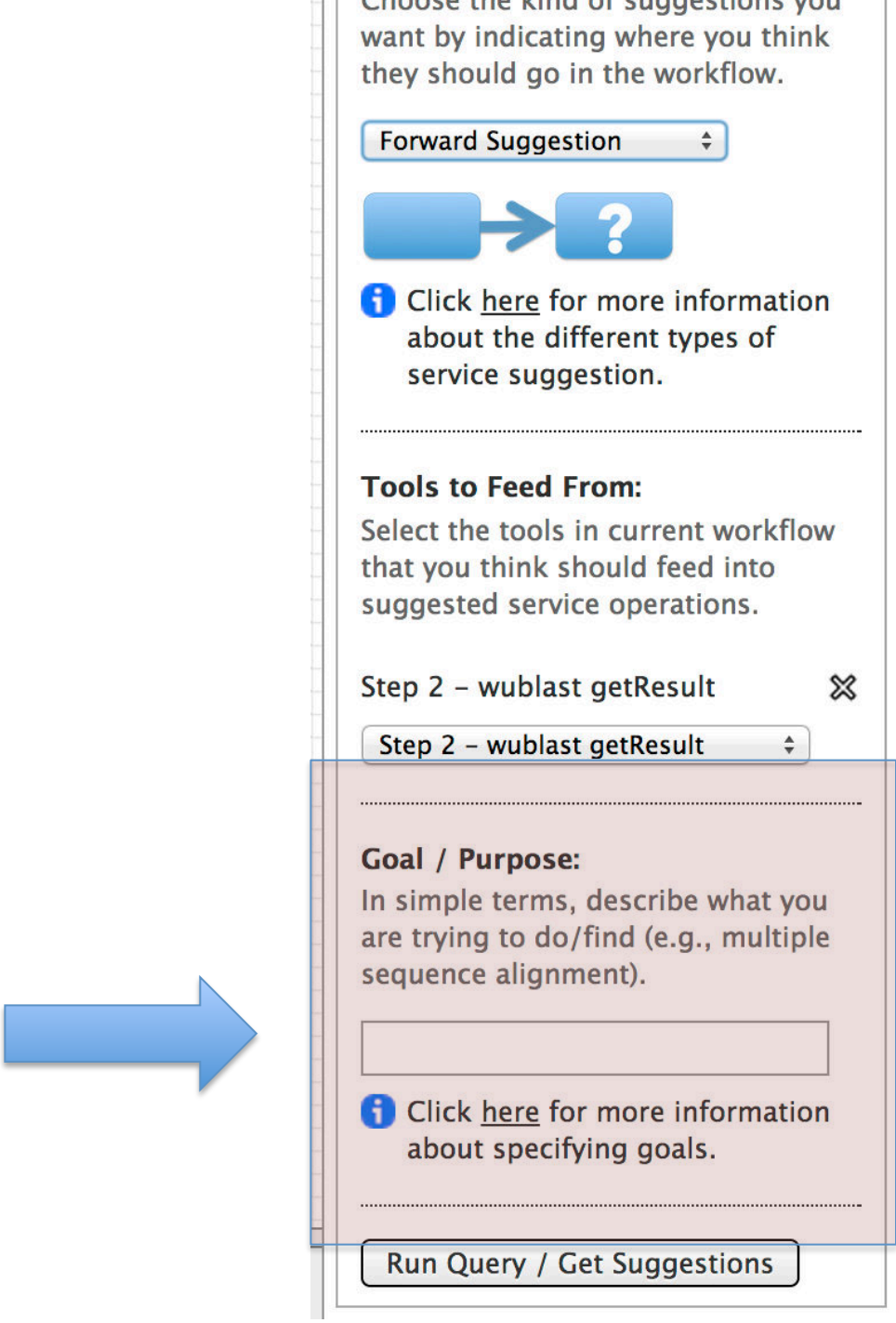


Service Suggestion

1. Choose the type of suggestion you want

2. Select relevant tools

Optionally, specify a goal



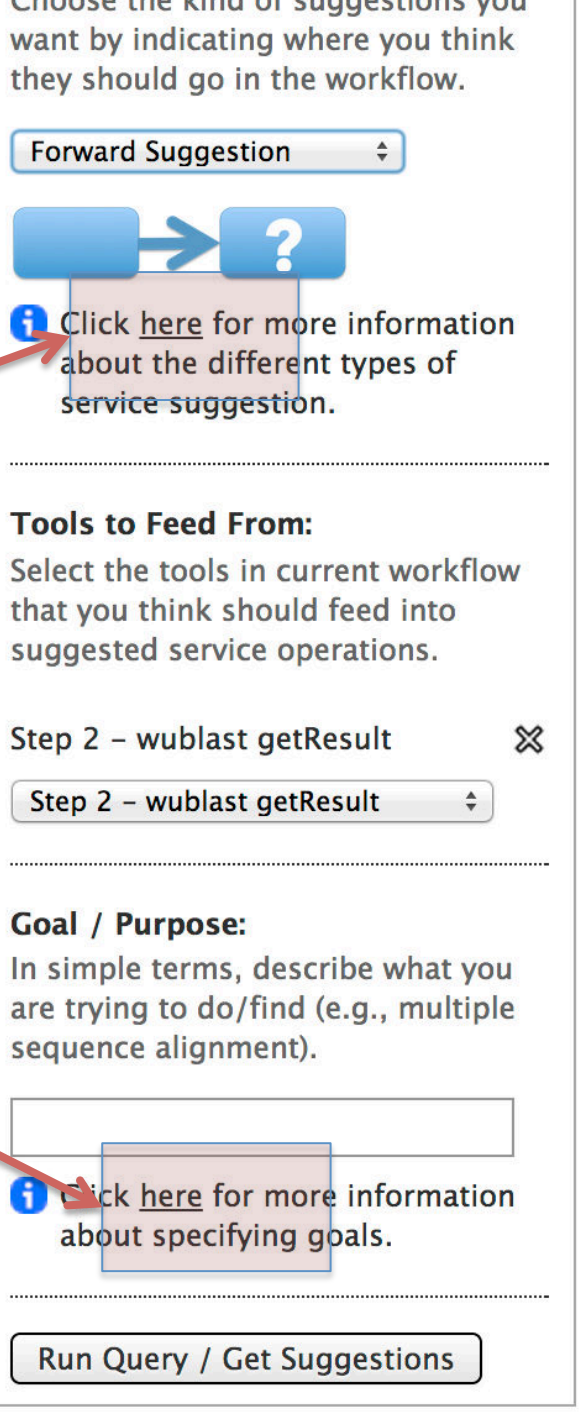
Service Suggestion

1. Choose the type of suggestion you want

2. Select relevant tools

Optionally, specify a goal

If you're not sure what something means then click on "help" to display a modal help dialog.



Service Suggestion

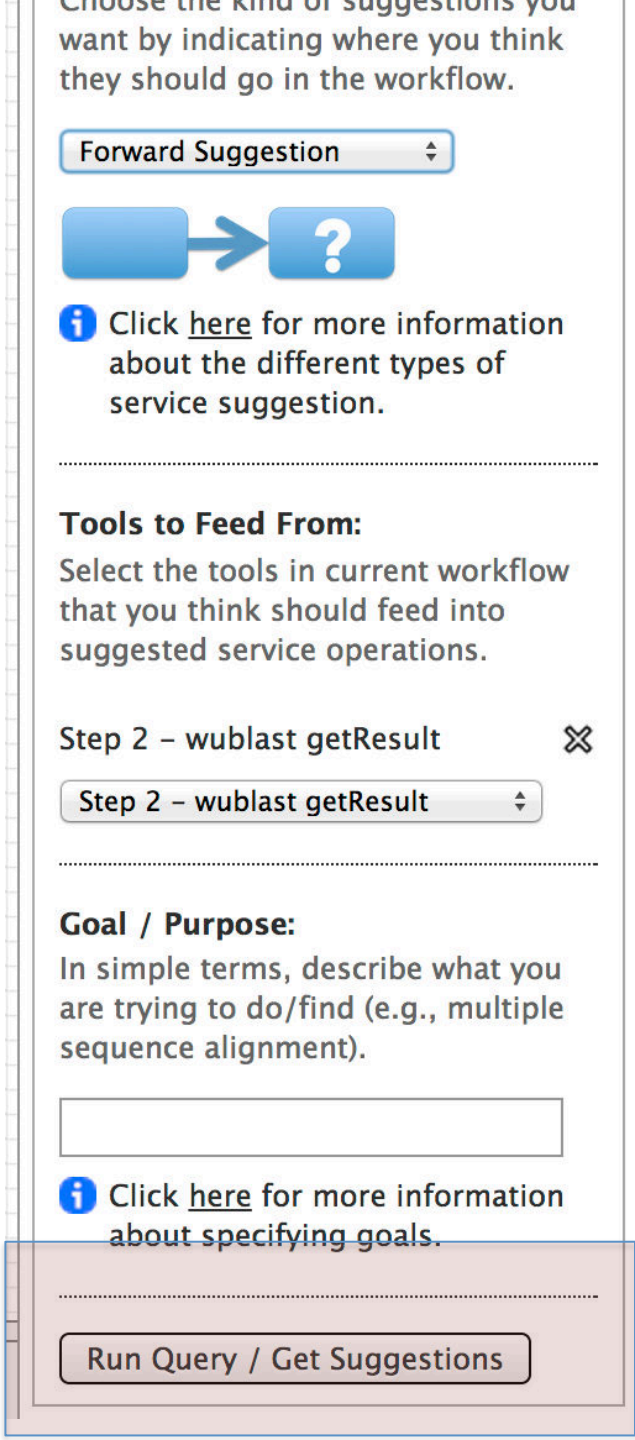
1. Choose the type of suggestion you want

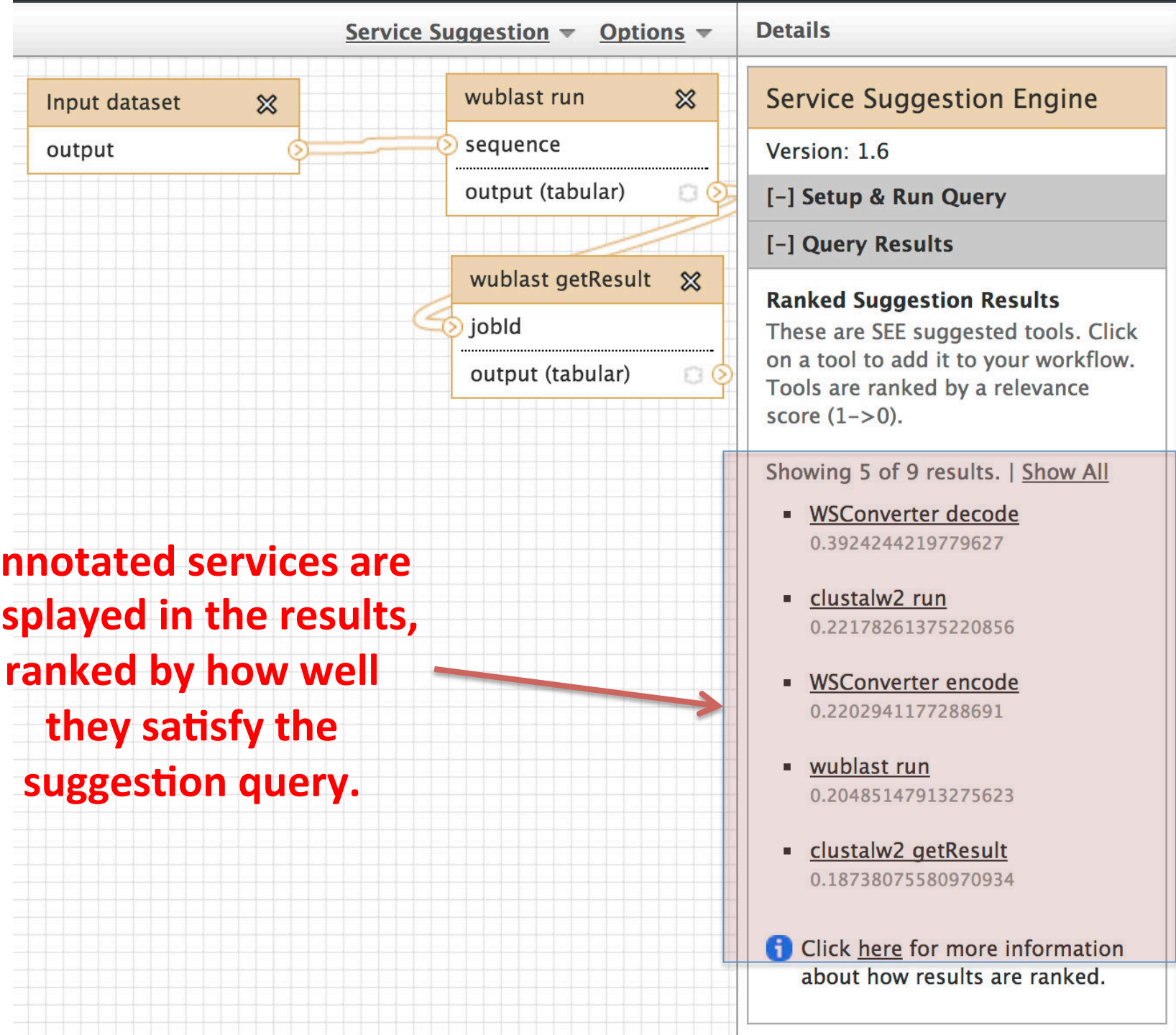
2. Select relevant tools

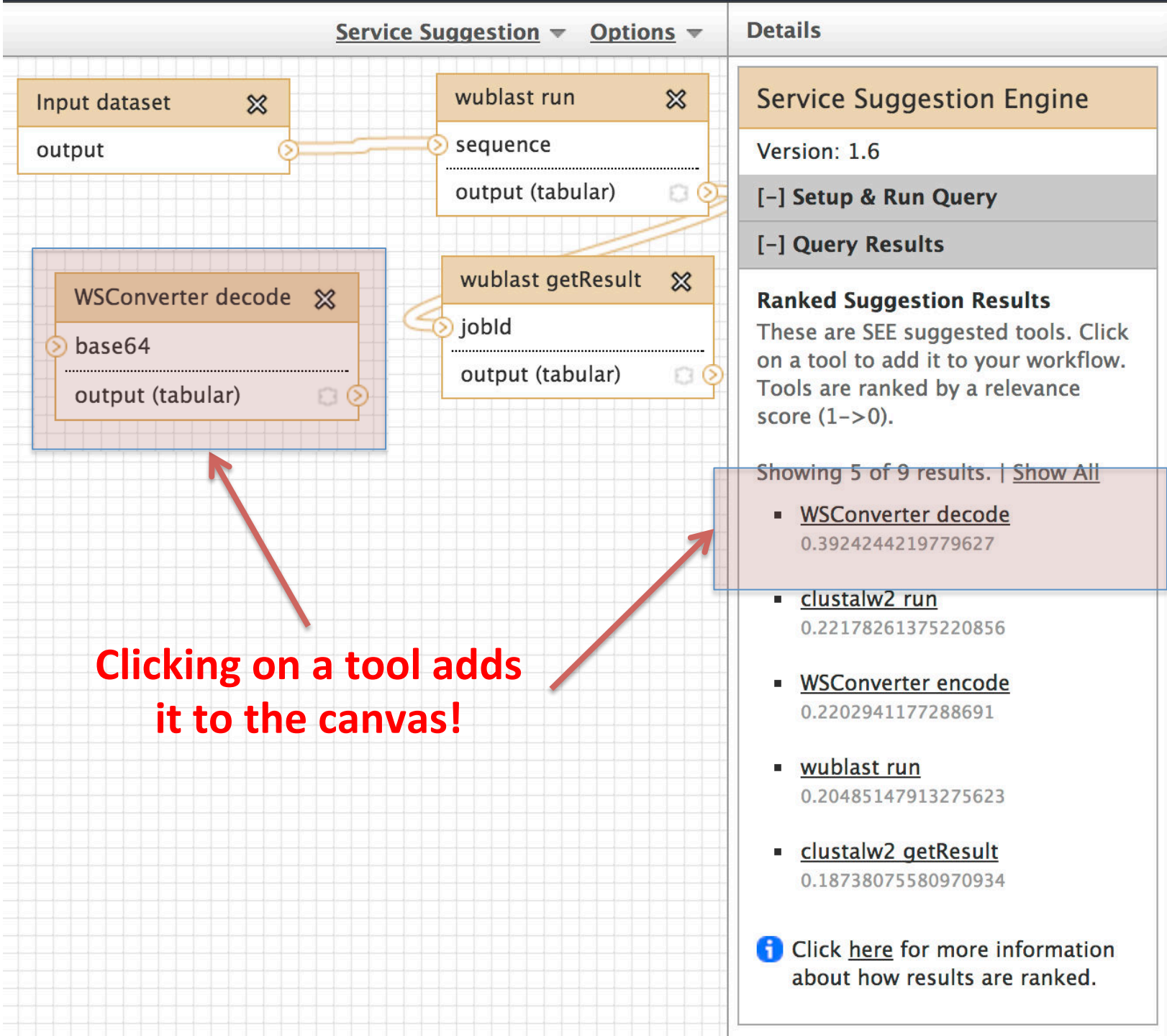
Optionally, specify a goal

3/4. Run the query to get suggestions!

Once you've specified what you want, click on "Run Query" to get suggestions




Service Suggestion
Options
Details
Input dataset
output
wublast run
sequence
output (tabular)
wublast getResult
jobId
output (tabular)
Service Suggestion Engine
Version: 1.6
[–] Setup & Run Query
[–] Query Results
Ranked Suggestion Results
These are SEE suggested tools. Click on a tool to add it to your workflow. Tools are ranked by a relevance score (1–>0).
Showing 5 of 9 results. | Show All
WSConverter decode
0.3924244219779627
clustalw2 run
0.22178261375220856
WSConverter encode
0.2202941177288691
wublast run
0.20485147913275623
clustalw2 getResult
0.18738075580970934
Click here for more information about how results are ranked.
Annotated services are displayed in the results, ranked by how well they satisfy the suggestion query.

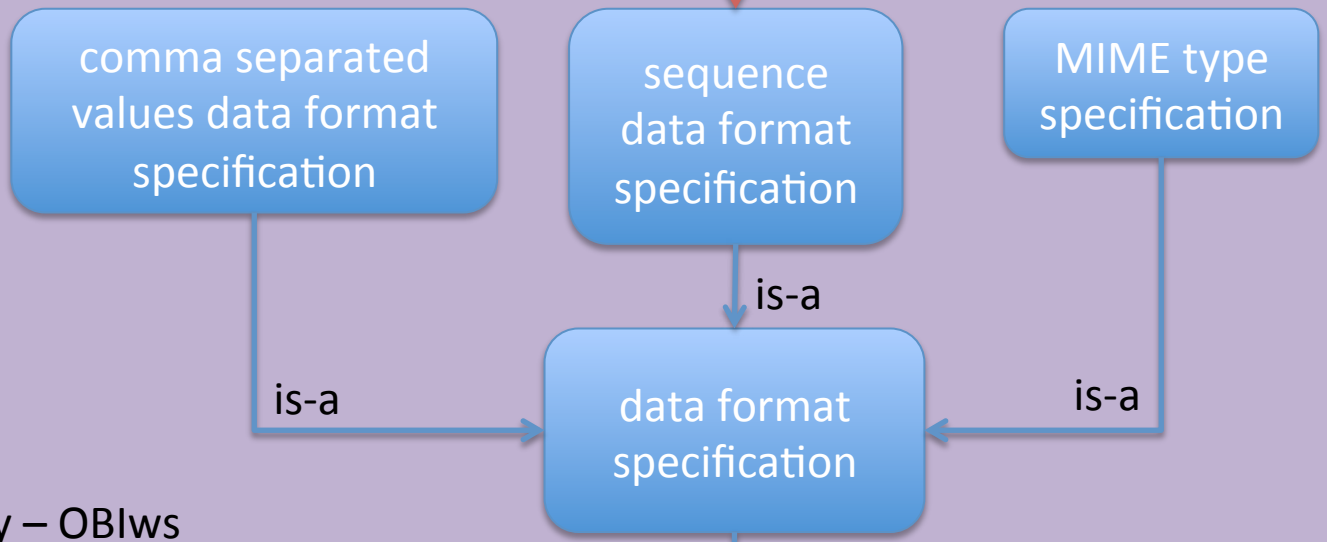

Service Suggestion
Options
Details
Input dataset
output
wublast run
sequence
output (tabular)
WSConverter decode
base64
output (tabular)
wublast getResult
jobId
output (tabular)
Service Suggestion Engine
Version: 1.6
[–] Setup & Run Query
[–] Query Results
Ranked Suggestion Results
These are SEE suggested tools. Click on a tool to add it to your workflow. Tools are ranked by a relevance score (1–>0).
Showing 5 of 9 results. | Show All
WSConverter decode
0.3924244219779627
clustalw2 run
0.22178261375220856
WSConverter encode
0.2202941177288691
wublast run
0.20485147913275623
clustalw2 getResult
0.18738075580970934
Click here for more information about how results are ranked.
Clicking on a tool adds it to the canvas!

Why not annotate Galaxy Tools to enable the SSE?

tabular_to_fasta.xml – Example of a Semantically Annotated Galaxy Tool

```
<description>converts tabular file to FASTA format</description>
<command interpreter="python">tabular_to_fasta.py $input $title_col $seq_col $output </command>
<inputs>
    <param name="input" type="data" format="tabular" label="Tab-delimited file"/>
    <param name="title_col" type="data_column" data_ref="input" multiple="True" numerical="False" label="Title column(s)" help="Multi-
        select list - hold the appropriate key while clicking to select multiple columns"/>
    <param name="seq_col" type="data_column" data_ref="input" numerical="False" label="Sequence column" />
</inputs>
<outputs>
    <data name="output" format="fasta" modelReference="http://purl.obolibrary.org/obo/OBIws_0000106" />
</outputs>
```

All we need to do is add modelReferences to a tool's XML file!

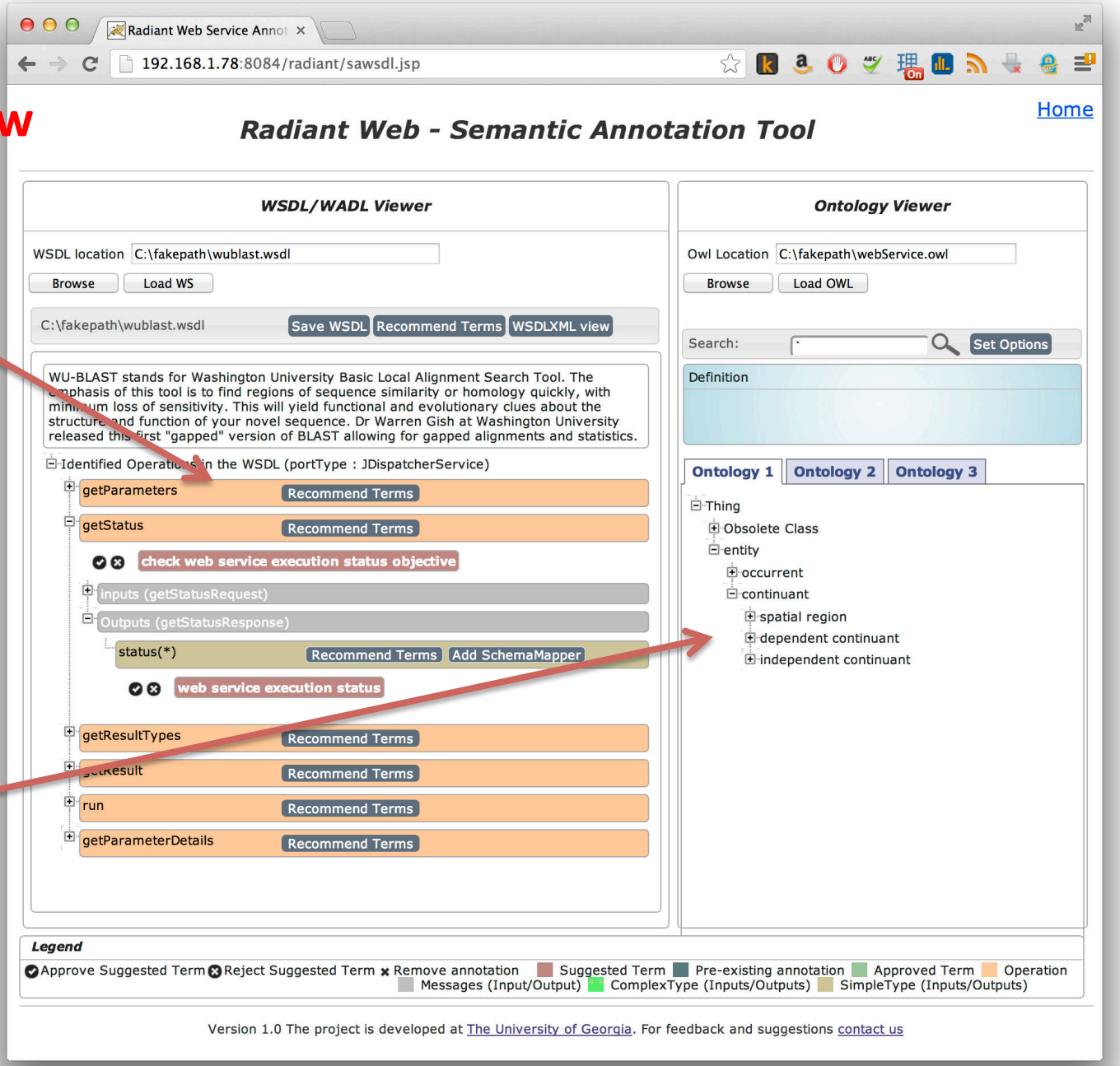


Ontology – OBIws

Annotating Services with RadiantWeb

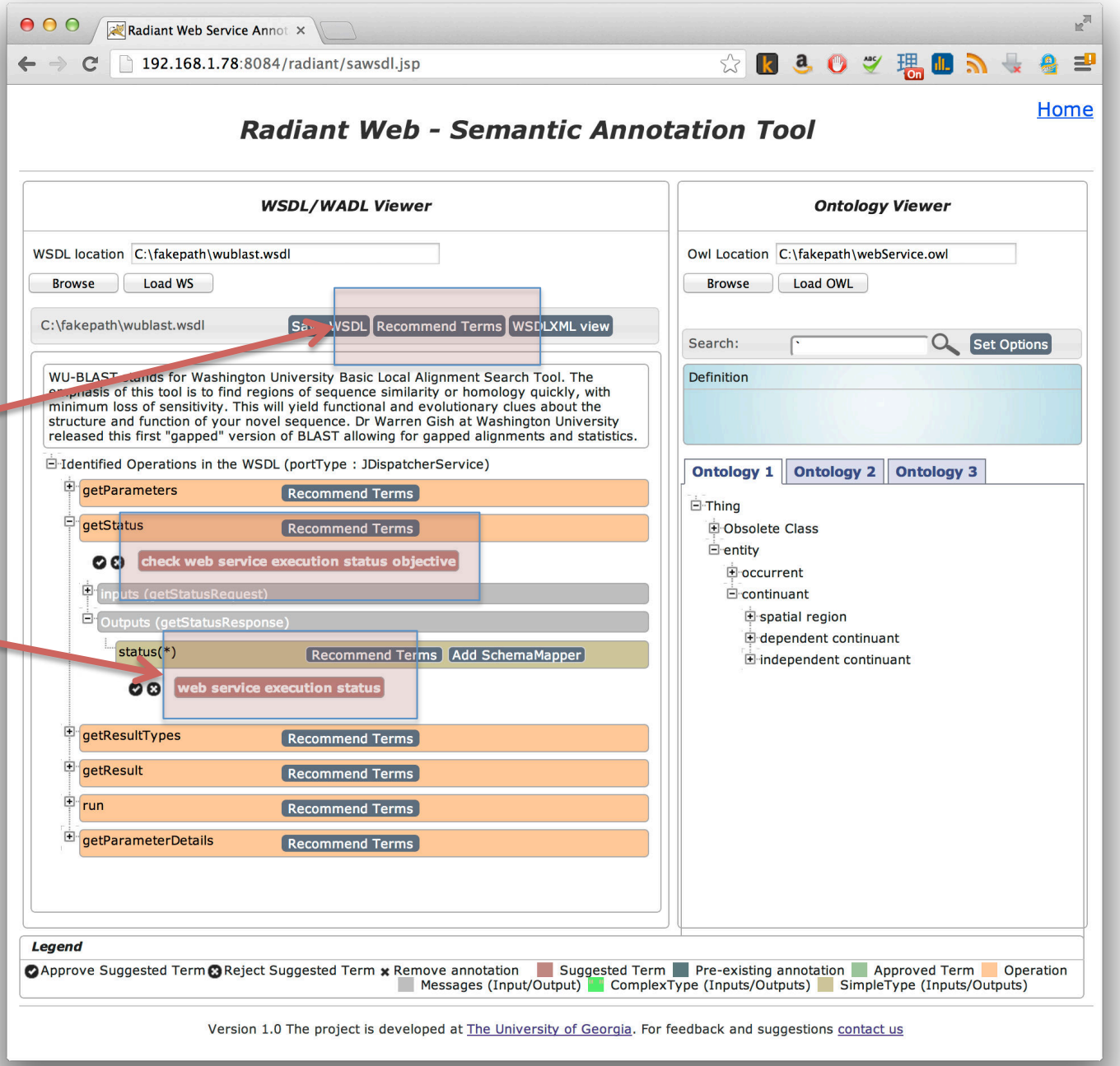
Simplified View of XML File

Tree View of Ontology



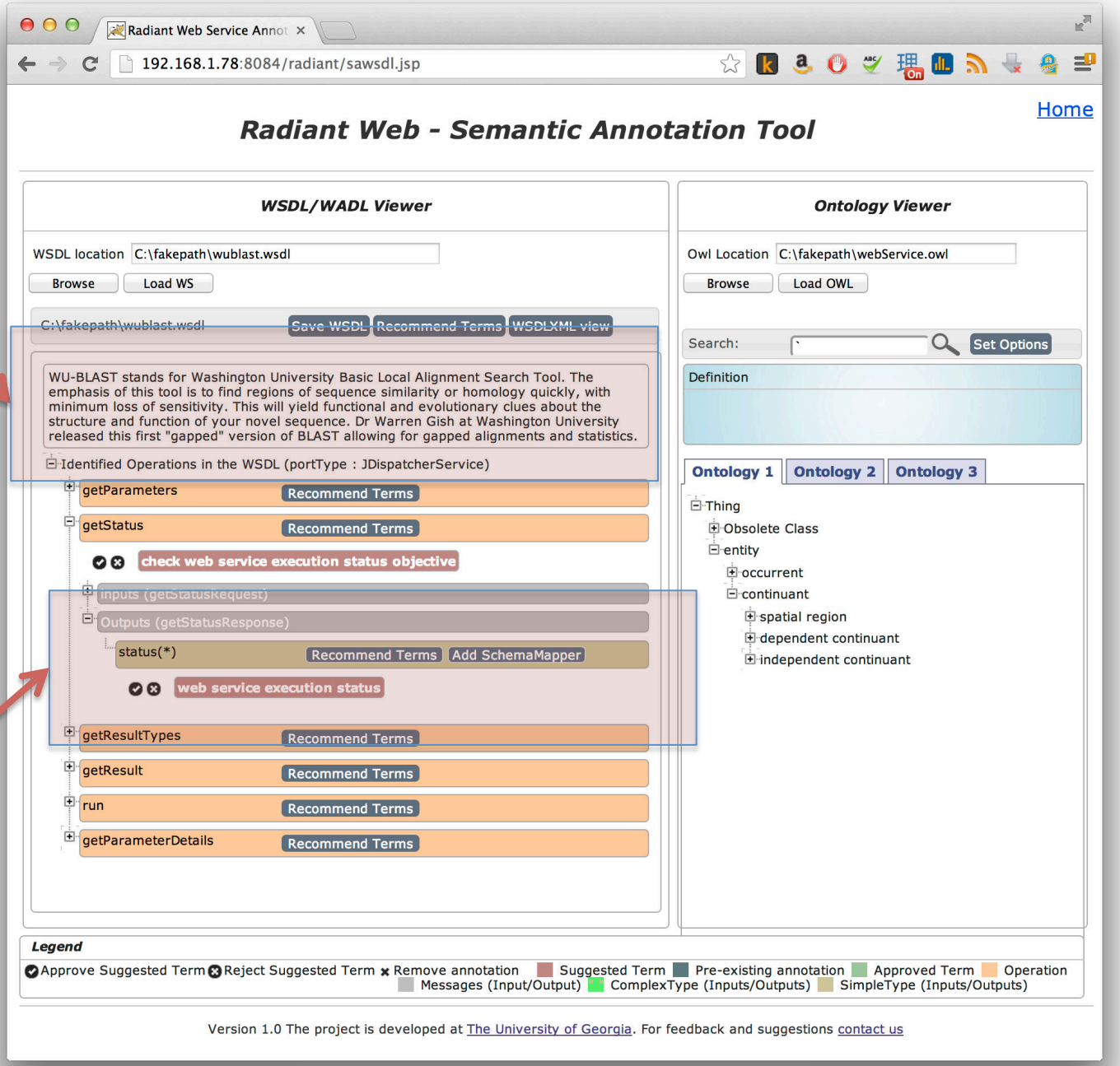
Annotating Services with RadiantWeb

Annotation Recommendations



Annotating Services with RadiantWeb

Documentation



Inputs/Outputs

Adding Web services to Galaxy

Advantages

- Increased tool/database access
- Don't need to wrap the tools/data access
- Distribute the load - Utilize someone else's computers
- Further empower the end user

Disadvantages

- Finding the Web services
- Moving data
- Hidden analysis step (Get job ID)
- All possible result formats (many not compatible with existing Galaxy tools)
- Security
- Banned from sites (depends on who is viewed as the user)

Adding a Semantic Suggestion Engine

Advantages

- Helps users find Galaxy tools with the desired functionality
- Helps with workflow construction
- Annotated tools are better documented tools. You will now what that parameter does and understand inputs and outputs

Disadvantages

- The community needs to annotate its tools
- Not all semantic terms will exist
- You give up some display area in the history column when the SSE is being used. It can be collapsed when not in use.

Thank you!

http://mango.ctegd.uga.edu/jkissingLab/SWS/