Taverna Xpath service
Getting Data out of XML

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The Basics of XML

- XML – e**X**tensible **M**arkup **L**anguage
- Designed for the storage and transport of data
  - This includes passing data between services or retrieving data from a Web page
- Provides a machine readable dataset
- Many service providers export data in XML

Example

```
<?xml version="1.0"?>
<note>
    <to>Katy</to>
    <from>Helen</from>
    <heading>Reminder</heading>
    <body>Don't forget about Bonn Trip!</body>
</note>
```

- The following website has lost of information about XML and tutorials: http://www.w3schools.com/xml

Extracting XML Elements

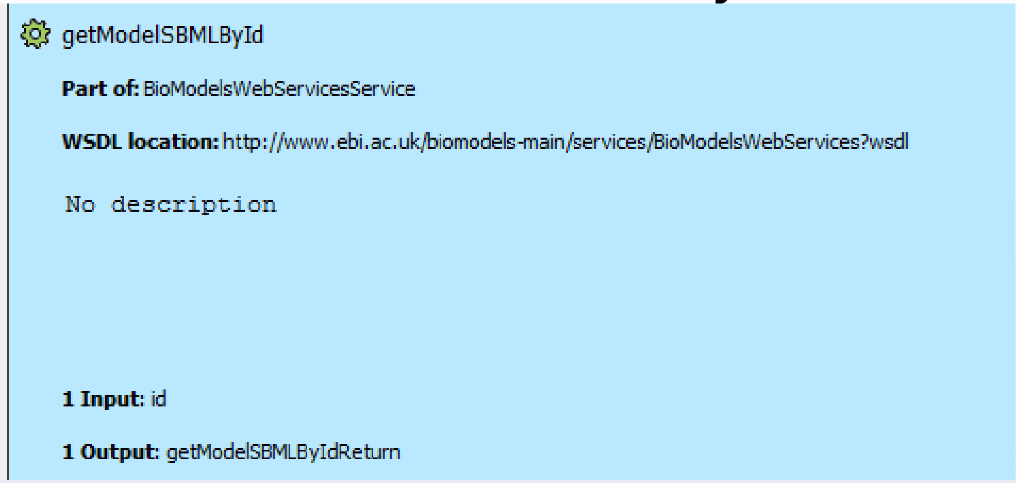
- Often, we need to extract particular elements of the XML to feed into the next services in the workflow
- Taverna has a dedicated service to help you do this
- Go to the service panel and find "Xpath Service" in the *Service Templates* section.
- We will use this service to explore the contents of an SBML file from the BioModels database, but first we need to find the BioModels services

Extracting XML Elements from SBML

- SBML is the Systems Biology Mark-up Language. It is the community standard for describing systems biology models
- SBML models contain information about the reactions between enzymes, genes, and metabolites, and their interactions in living systems
- Well-annotated SBML models will contain descriptions of model entities and official IDs to link those entities back to their sources (e.g. Uniprot IDs for proteins/enzymes, KEGGIDs or ReactomeIDs for reactions etc)

Extracting XML Elements from SBML

- We will find all the BioModels constructed in yeast (*Saccharomyces cerevisiae*), and find the publications about them
- In Biocatalogue, search for the 'BioModels':
  - *getModelsIDByTaxonomy*
  - *getModelSBMLByID*
- And add these services to the Service Panel and your workflow.
  - Hint: As you did in the REST exercise



getModelSBMLById

Part of: BioModelsWebServicesService

WSDL location: http://www.ebi.ac.uk/biomodels-main/services/BioModelsWebServices?wsdl

No description

1 Input: id

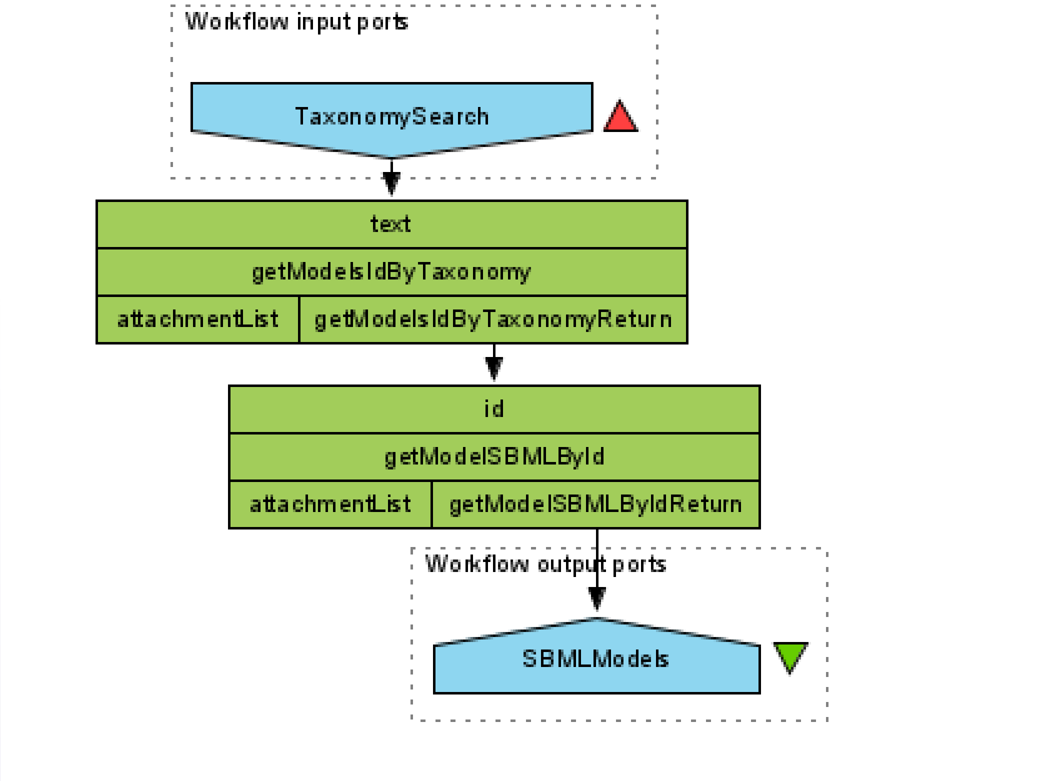
1 Output: getModelSBMLByIdReturn

Extracting XML Elements from SBML

- Add a input port (rename the service to TaxonomySearch) and connect it with getModelsIdByTaxonomy
- Then connect the output (Return) from getModelsIdByTaxonomy with the input for getModelSBMLById
- Create an output port

Extracting XML Elements from SBML

- The workflow should look like this

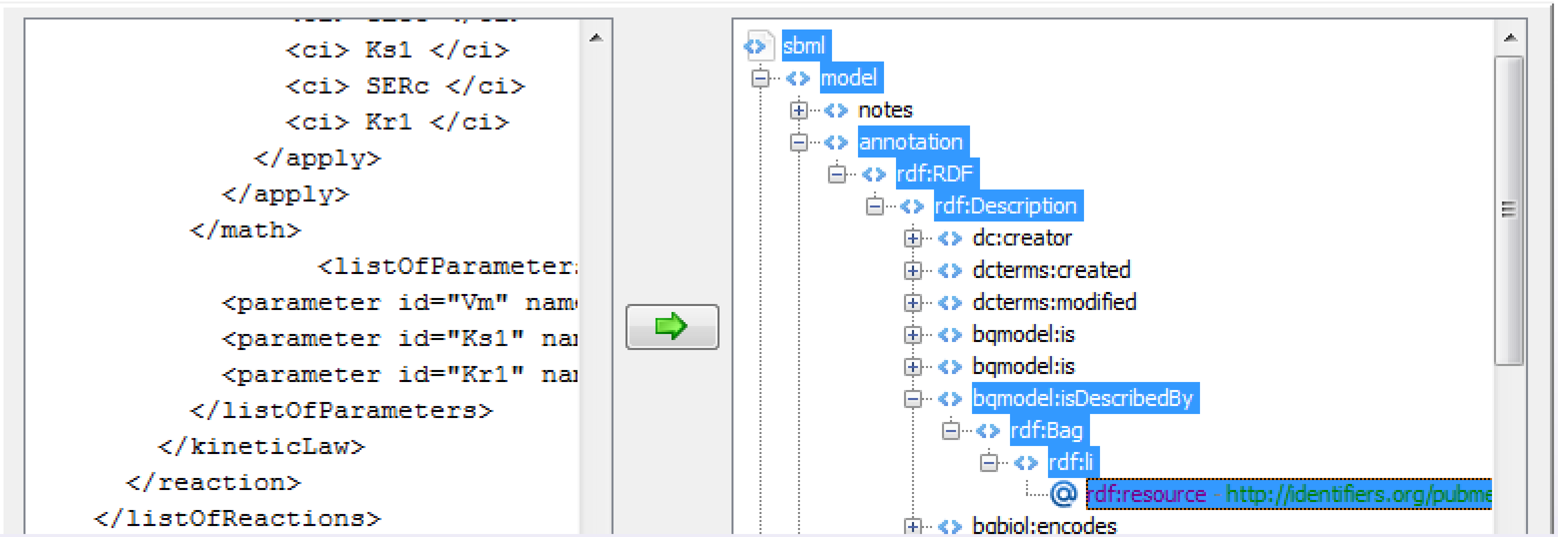


Extracting XML Elements from SBML

- Run the workflow using the value ***Saccharomyces cerevisiae***
  - *Hint: As you only need 1 Value you can "Cancel" the workflow as soon as a few Values appear*
- Save one of the SBML models as an XML file
  - Hint: In the results view select on of the Values from the List for example "Value 1"
  - Click on "Save Value"
    - Using a .xml file extension will make it easier to find

Extracting XML Elements from SBML

- Now import the Xpath Service from Taverna
- In the pop-up window, enter the path to the saved SBML file and click the green arrow to load it into the service
- By expanding the + icons, you can explore the file
- Expand the XML under ‘annotation’, until you reach RDF:resource

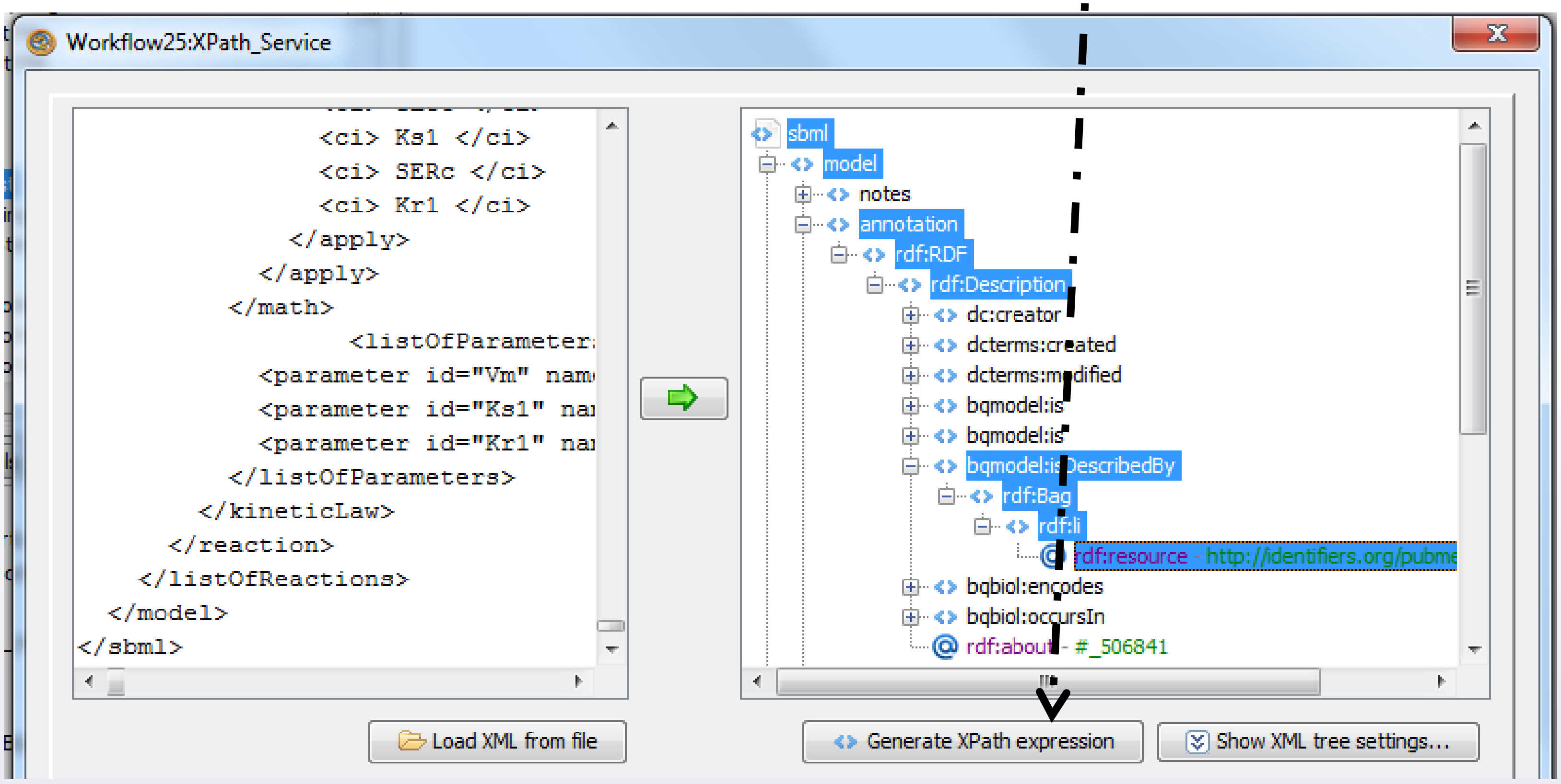


```
                <ci> Ks1 </ci>
                <ci> SERc </ci>
                <ci> Kr1 </ci>
              </apply>
            </apply>
          </math>
                  <listOfParameter:
            <parameter id="Vm" nam
            <parameter id="Ks1" na
            <parameter id="Kr1" na
          </listOfParameters>
        </kineticLaw>
      </reaction>
    </listOfReactions>
```

```
sbml
  model
    notes
    annotation
      rdf:RDF
        rdf:Description
          dc:creator
          dcterms:created
          dcterms:modified
          bqmodel:is
          bqmodel:is
          bqmodel:isDescribedBy
            rdf:Bag
              rdf:li
                rdf:resource - http://identifiers.org/pubme
          bqbiol:encodes
```

Extracting XML Elements from SBML

- □ Click on ‘Generate Xpath From Expression’
- □ Then Click on ‘Run Xpath’ and click ‘Apply’
- □ This service will now pull out all the reactions from each model



```
            <ci> Ks1 </ci>
            <ci> SERc </ci>
            <ci> Kr1 </ci>
          </apply>
        </apply>
      </math>
          <listOfParameter:
        <parameter id="Vm" nam
        <parameter id="Ks1" na
        <parameter id="Kr1" na
      </listOfParameters>
    </kineticLaw>
   </reaction>
  </listOfReactions>
 </model>
</sbml>
```

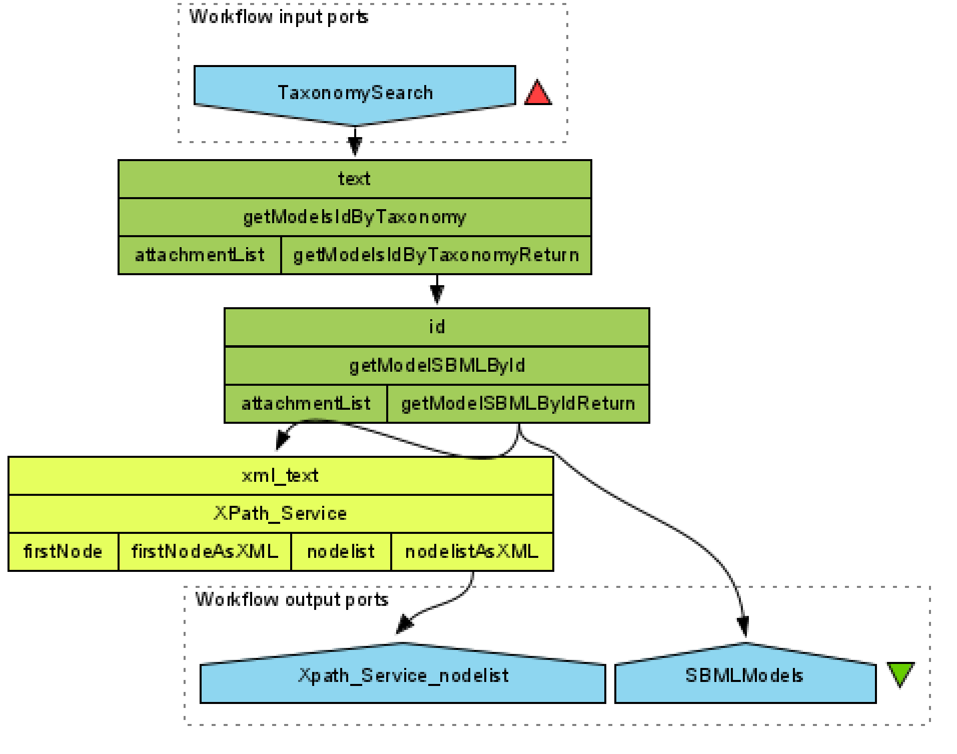
```
sbml
  model
    notes
    annotation
      rdf:RDF
        rdf:Description
          dc:creator
          dcterms:created
          dcterms:modified
          bqmodel:is
          bqmodel:is
          bqmodel:isDescribedBy
            rdf:Bag
              rdf:li
                rdf:resource - http://identifiers.org/pubme
          bqbiol:encodes
          bqbiol:occursIn
          rdf:about - #_506841
```

Extracting XML Elements from SBML

□ Connect it to the output of ‘*getModelSBMLByID’*

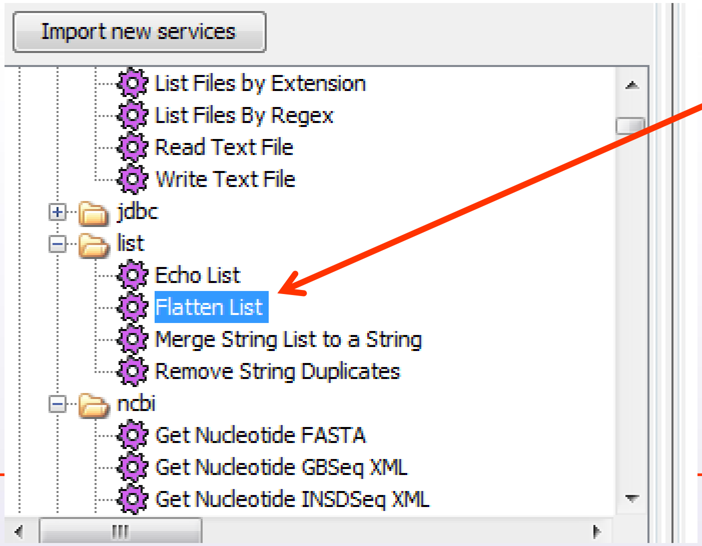
□ Add an output port to the Xpath service “nodeListAsXML”

□ Save and run the workflow again



Extracting XML Elements from SBML

- We can change the output of the Xpath service into a flattened list
- (In Design View) Go to the Services Panel and add a Flatten List (from “Available Services”/Local Services”/“list”)

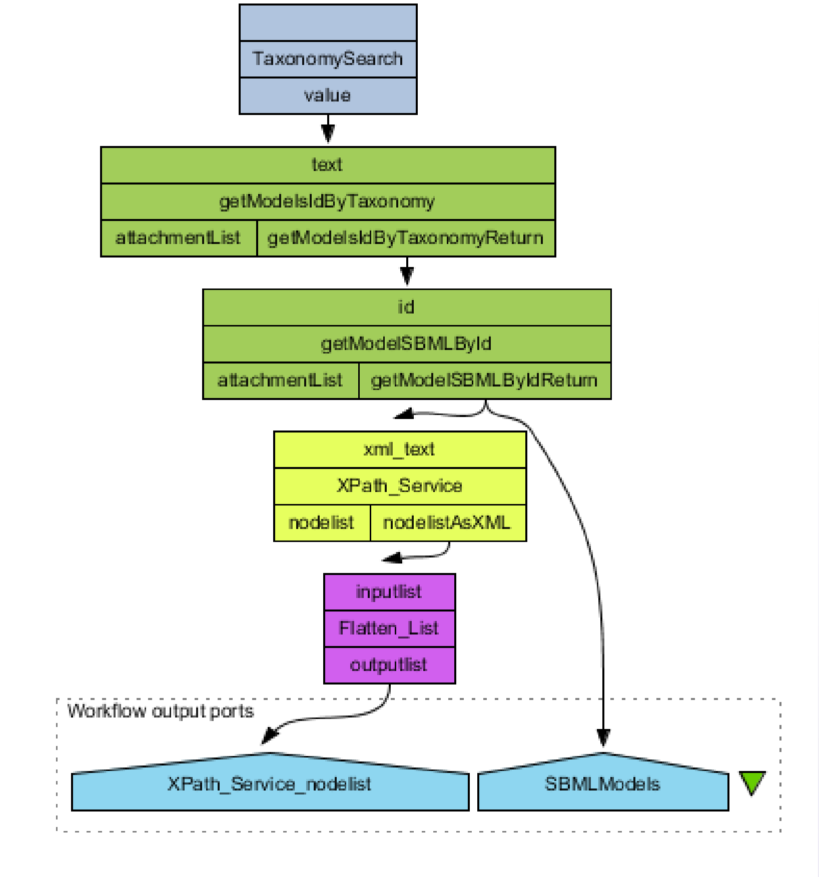


Import new services

List Files by Extension
List Files By Regex
Read Text File
Write Text File
jdbc
list
Echo List
Flatten List
Merge String List to a String
Remove String Duplicates
ncbi
Get Nucleotide FASTA
Get Nucleotide GBSeq XML
Get Nucleotide INSDSeq XML

Extracting XML Elements from SBML

- □ Connect the output of the Xpath service to the “Flatten List”
- □ Connect the output of the “Flatten List” with the output port



Extracting XML Elements from SBML

- Run the workflow again
  - Note: Flatten_List will not show any values until the workflow is finished as its output is a single list
- Optional: Try the service with a different Xpath Query
  - In Design View right click the Xpath Service
  - Select Configure Xpath Service
  - This brings back up the configuration Screen you saw earlier.