

An Introduction to Designing and Executing Workflows with Taverna

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Workflows

- Sophisticated analysis pipelines
- A set of services to analyse or manage data (either local or remote)
- Data flow through services
- Control of service invocation
- Iteration
- Automation
- Access to intermediate results





Workflows in Taverna

- This tutorial will give you a basic introduction to designing, and reusing workflows in Taverna and some of its main features.
- Workflows in this practical use small data-sets and are designed to run in a few minutes. In the real world, you would be using larger data sets and workflows would typically run for longer
- Taverna allows you to use different forms of data input and save output data in different formats too – we will look at that in this tutorial as well.









Taverna Workbench





Workflow Diagram

- The **workflow diagram** is the visual representation of the workflow, it:
- Shows inputs, outputs, services and data flows
- Allows editing of the workflow by dragging and dropping and connecting services together
- Enables saving of workflow diagrams for publishing and sharing









Workflow Diagram

Taverna understands difference types of services

Туре	Description	Туре	Description
Beanshell	A user editable scripting operation using Beanshell script	Local_service	A standard Beanshell
Nested_workflow	A sub-workflow exposed as a single operation	wsdl_web_service	A processor accessing a standard SOAP service
Rshell	A user editable script in R	REST_Service	A processor accessing a RESTful web service
SpreadsheetImport	An operation for loading spreadsheet data in CSV and Excel format	Tool_service	Calling a local or remote tool/script
String_constant	A single constant string	Interaction	Interaction in a web browser
XPath_Service	Extraction of data from XML data	Component	Re-usable component workflow











Workflow Diagram

Taverna workflows also have

Element	Description
input_port	Input port
output_port 🗸	Output port
\sim	"Merge" - make a list out of elements (often sub-lists)
XML_splitter	XML Splitter
Ŧ	Data flow
5	Control flow (run after)



Workflow Explorer

- The **Workflow Explorer** shows the detailed view of your workflow. It shows default values and descriptions for service inputs and outputs and it shows where remote services are located. It also shows configuration details, such as iteration and looping
- Workflow validation details can also be found here. Before a workflow is run, Taverna checks to see if it is connected correctly and if its services are available.









Updates and Plugin Installation

- It's a good practice to update Taverna regularly
- Taverna updates are issued on a regular basis
- There is also a number of plugins which are developed for Taverna
- To get the updates and plugins select Advanced -> Updates and plugins

S Updates and plugins	×
Common services 2.5.0-20140415	Uninstall
Taverna 2 common services	Update
Component Service 2.5.0-20140415	Update all
Create and use components, wrapping underlying workflows	
Interaction Service 2.5.0-20140415	
Web-based user interactions during workflow run	
Workbench (required) 2.5.0-20140415	
Taverna 2 workbench. Required for graphical interface.	
Find Updates Find New Plugins	Close



Available Services Panel

Lists services available by default in Taverna

- Local services a standard set of utilities
- WSDL Web Service secure and public
- RESTful Services
- R Processor services (for statistical analyses)
- Beanshell scripts
- XPath scripts
- Spreadsheet import service
- Interaction service allows the workflow to "ask" for information in a web browser
- Component re-usable workflows

The services panel also allows you to add new services from the web or from file systems – there are loads more available!



- We will start with something easy we will use an Allen Brain service to retrieve information about the experiments for a gene whose name we will provide
- Go to the <u>www.biocatalogue.org</u> and search for "Allen brain"

BioCatalogue	
Search: allen brain	Gol Home & Services O Register
Home »	
	The BioCatalogue: providing a curat
Helpful Links	BioCatalogue currently has 2491 service
Catting started with the Catalogue	



• From the results select Allen Brain Atlas Browse

Search query " alle	en brain" returned 3 items
Services (2)	Service Providers (1)
Allen Brain	Atlas Browse REST
Browse the Alle	n Brain Atlas (<u>http://www.brain-map.org/</u>). User specifies the model, model id and format for result (json, xml, csv).
Previden esi ba	
Provider: api-br	<u>in-map-org</u> Base URL: <u>http://api.brain-map.org/api/v2/data</u>
MouseGen	eSearch SOAP
Data Retrieval	Identifier Retrieval Image Retrieval
The service allo	ws you to retrieve data (e.g mouse gene) from the Allen Mouse Brain Atlas, an interactive genome-wide image database of gene expression.
project website	http://mouse.brain-map.org/weicome.do
Provider: Allen	stitute for Brain Science WSDL Location: http://mouse.brain-map.org/services/GeneSearchService?wsdl



• Have a look at the service description

Overview Rest Services (4) Examples	Monitoring	History	
Provider: api-brain-map-org				
Location: Lowell, United States 🛛 🚟				
Submitter/Source:	? months ago)			
Base URL: http://api.brain-map.org/api/v2/data	I			
Documentation URL(s):				
http://help.brain-map.org/display/	api/RESTful+Model+,	Access+%28RM/	<u>4%29</u>	by 🗟 <u>Michael Cornell</u> Curator (2 months ago)
				Login to add a documentation URL
Description(s):				
Browse the Allen Brain Atlas (<u>htt</u> model id and format for result (jso For example, <u>http://api.brain-map</u>	<u>p://www.brain-map.or</u> m, xml, csv). .org/api/v2/data/Chro	<u>g/</u>). User specifie mosome/12.json	s the model,	by <u>B</u> Michael Cornell Curator (2 months ago)

Login to add a description



- Select the Rest Services tab and see how the service can be used
- Click on GET SectionDataSets

Jverview Re	t Services (4) Examples Monitoring History
What is an endpo	nt?
Quick Browse	GET SectionDataSets GET SectionImages Download Images GET /{Model}/{Modelld}.{resultFormat}
GET SectionDa	aSets GET /query.xml?criteria=model∷SectionDataSet,rma∷criteria,genes%5Bacronym\$eq%27{gene}%27%5Dν
Part of Service: Al	in Brain Atlas Browse
Part of Endpoint G	oup: none
Template: (2) http No description(s) y	/api.brain-map.org/api/v2/data/query.xml?criteria=model::SectionDataSet,rma∷criteria,genes%5BacronymSeq%27{gene}%27%5D#_rows=2 if
Tags on this end	bint: none
GET SectionIm Part of Service: <u>Al</u> Part of Endpoint G	ges <u>GET /query.xml?criteria=model::SectionImage,rma::criteria,%5Bdata_set_id\$eq{data_set}%5D&num_rows=2 In Brain Atlas Browse oup: none</u>
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- This service returns the results for a gene name that we will provide, and limits the number of results to 2
- We can copy the Template

<u>http://api.brain-</u> <u>map.org/api/v2/data/query.xml?criteria=model::SectionDataSet,rma::crite</u> <u>ria,genes%5Bacronym\$eq%27{gene}%27%5D&num_rows=2</u>

- In Taverna Workbench go to the Services Panel in the Design view
- From the Available Services select Service Templates and REST
- Right-click on it and select **Add to workflow** (see the next slide)



Import new services	
Constructed templates	
Beanshell – A service that allows Beanshell scripts, with dependencie	s on libraries
Interaction	
🐲 Nested workflow - A service that allows you to have one workflow ne	sted within another
🔚 REST Service – A generic REST service that can handle all HTTP met	ode
🕼 Rshell – A service that allows the calling of R scripts on an R server	REST Service
SpreadsheetImport - A service that imports data from spreadsheet:	Add to workflow
袋 Text constant - A string value that you can set	Add to workflow with name
🌍 Tool – A service that allows tools to be used as services	
XPath Service - Service for point-and-click creation of XPath express	ions for XML data
e	n
Workflow explorer Details Validation repor	t



0	8	Workflow3:REST_Service	x
	General Advanced		
	(1) HTTP Method:	GET	
	(1) URL Template:	http://api.brain-map.org/api/v2/data/query.xml?criteria=model::Sect	tic
	Preferred MIME type for data	a to be fetched from the remote server	
	() 'Accept' header:	application/xml	
		Help Apply Close	2

• Enter the template you copied into the URL template field:

http://api.brain-

map.org/api/v2/data/query.xml?criteria=model::SectionDataSet,rma::criteria,gene
s%5Bacronym\$eq%27{gene}%27%5D&num_rows=2



• Let's change the name of the service to: *AllenExperimentsForGene*





At the top of the workflow diagram panel, change the view to show all ports by clicking on the icon shown below



This view allows you to see any data input/output or parameter value options for your chosen service



- In a blank space in the workflow diagram, right-click and select Workflow input port from the Insert section
- Type in a name for this input (e.g. gene) and click OK

Do the same to create a new workflow output.
 Call this output *experiments*

Edit	
	Paste Ctrl+V
	Show details
	Annotate
	Show validation report
i	Create nested workflow
Inse	ert
	Workflow input port
$\mathbf{\nabla}$	Workflow output port
9	Beamsner
3	Interaction
i	Nested workflow
REST	REST
R	Rshell
نې	Spreadsheet import
<i>ت</i> ې	Text constant
G	Tool
\mathbf{O}	XPath





- Connect the input and output ports
- Your workflow should look like this





 Run the workflow by selecting File -> Run workflow, or by clicking on the play button at the top of the workbench

(3
F	File Edit Insert View Workflows Components Advanced Help
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[📝 Design 🖩 Results ໜ myExperiment 🔇 Service Catalogue
ſ	Service panel
L	Filter: protein
	Import new services
	Comparison Matching services
L	Eccal services
	Get Protein FASTA



• You'll get a pop up window where you can enter the data for the workflow.

000	Input values for 'Workflow48'
Diagram	sciName
Restor que poli- tica que poli- para en de construir en de con	Port description No port description
-Workflow description	Example value No example value
No description	X Delete 🔊 Set file location 🚱 Set URL
	Set the input value
-Workflow author No author	
	Drag to re-arrange, or drag files, URLs, or text to add
	Load previous values







8		Taverna	Workbench Core 2.5.0		- 🗆 ×	
File Edit Insert View Workflows Components Advanced Help						
📝 Design 🛗 Results my myExperiment	🕼 Design 🛗 Results 🚾 myExperiment					
	Graph Progress report					
at la state at la						
Click on a run to see its values Click on a service in the diagram						
to see intermediate values (if available)					Window	
Workflow3 2014-07-13 17:53:23				•		
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			·····			
			Allen Experimente For Cone ¹			
			AllenExperimentsForGene			
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	Finished Pause	X Cancel	⅔ Edit executed workflow	🍫 Refresh intermediate values	Show workflow results	
Workflow results					🕞 Save all values	
A cape V experiments						
	¥	Value type Text	V Refresh 🗌 Wrap text		🔚 Save value	
					^	
		<pre><response <section_data_set="" s="" success="true"></response></pre>	start_row='0' num_rows='2' tota1_rows='1	5'> <section-data-sets></section-data-sets>		
		<pre></pre>	ue"/>			
	<pre><delegate>true</delegate></pre>					
	<expression>true</expression>					
	<failed>failed>failed></failed>					
	<pre><failed-facet>734801840</failed-facet> </pre>					
		<pre><qreen-channel file="true"></qreen-channel> </pre>				
		<pre>classes/id/ chame nil="true"/></pre>				
	<plane-of-section-id>2</plane-of-section-id>					
		<pre><qc-date>2009-09-24T10</qc-date></pre>	0:35:35Z		¥	

- You should see the workflow running
- Once the workflow finished running
- Click on experiments and Value to see the results



Let's save the workflow now as "experiments_for_gene"





Service ports

- Most of the time, you don't need to connect all ports. Some are optional and some already have default values set.
- Service documentation should tell you this. You can use the BioCatalogue to find documentation and user descriptions
- Change the orientation of the port names to fit them on the screen more easily by clicking on the icon shown below





Service ports

- Most of the time, you don't need to connect all ports. Some are optional and some already have default values set.
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Adding a Workflow Description

- In the **Design** view, right-click on a blank part of the workflow diagram and select **Annotate**
- Add some details about the workflow e.g. who is the author, what the workflow does
- You can also add examples and descriptions for the workflow inputs by selecting them and selecting **Annotate**
- Add an example for the gene *Adora2a*
- Save the workflow by going to "File -> save workflow"
- Run the workflow again and look at the results



Additional Exercise 1: Xpath Service

- This exercise is optional.
- Our workflow returns the result in the XML format.
- Taverna provides a service which helps to process XML data –
 XPath service
- Go to myExperiment and find *XPath service Tutorial*
- Using this tutorial try adding the XPath Service to the workflow to process the XML results



- We can add input data into the workflow not only manually but also from a file. Go to myExperiment pack and download the file *Genes for VPH-Share workshop*
- Click Run workflow again but instead of selecting Set value select Set file location and navigate to where you saved the file

Port description	000	Choose files	or directory
No port description		Data	*
	Name	A	Date Modified
Example value No example value	ebi_sequence	_configurable_iterati	Wednesday, November 27, 2013 7: Monday, November 25, 2013 5:36
X Delete abit Set value Set file location Set file set file location Www.myexperiment.c : http://www.myexperiment.c			
	Fil	le Format: All Files	\$



 Instead of downloading the file we can point the workflow to the file's URL (if we know it). Let's run the workflow again but this time select Set URL and paste in http://www.myexperiment.org/files/1213/download/genes.txt

🗶 Delete 🖓 Set value 🗎 S	et file loca	tion 🥹 Set URL
	2	
	Add an Set the	http URL
	Name:	http://www.myexperiment.org/files/1213/download/genes.txt
		OK Cancel



- So far we used simple text files but it is also possible to use spreadsheets as sources of input data. In order to do that we will need to add a Spreadsheet tool to our workflow.
- From the myExperiment group download the file *genes.xls* open it on your machine and see what it contains (the list of the genes is in cells B2 to B5)
- From the Service Templates select SpreadsheetImport rightclick on it and add it to the workflow



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📝 Design 📲 Results 🔤 myExperiment 🍌 XworX BIFI Perspective 🔇 Service Catalogue						
	Service panel					
Filter:	Clear					
Im	port new services					
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🔻 🗁 S	Service templates					
Beanshell – A service that allows Beanshell scripts, with dependencies on libraries						
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🎆 Nested workflow - A service that allows you to have one workflow nested within another						
REST Service - A generic REST service that can handle all HTTP methods						
Rshell - A service that allows the calling of R scripts on an R server						
SpreadsheetImport - A service that imports data from spreadsheets						
Dext constant - A string value that you can set						
	Tool – A service that allows tools to be used as services					



 In the pop up window set the correct range for columns and rows (untick the box "all rows")

	^		
۲	Spreadsheet Import Configuration	×	
Configur Select the	r e spreadsheet file im port data range		
Columns From B	to B		
Rows From 2	to 5 All rows Exclude header row		Workflow input ports
Empty cells			♦ gene
🖲 Use a	an empty string	lle	nExperimentsForGene
🔿 Use f	this value:	es	ponseBody status
⊖ Gene	rate an error value	- w	output ports ▼
		e	xperiments 🗸 🗸
	Cancel Next Finis	h	



- We need to delete the input port for the workflow (right click on it and select **Delete**)
- The Spreadsheet tool expects as an input the URL (or path) to the file. The best way to feed in that URL/path is to add a service called **Text constant**





 Where is says Add your own value here enter: http://www.myexperiment.org/files/1214/download/genes.xls (or if you prefer the full path to your local file), then Apply and Close

	a 🔿 🔿 🔿	Workflow48:Text_constant	ksa
>	Add your own val	ue here	
	ri		
	o		
	n		
	a		
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	1		Boc
			urei
	Line: 1 Column: 23		
		Load text Save text Clear text	
	ly .		
	n	Help Apply Clos	e



 Connect the Text constant with the SpreadsheetImport and the SpreadsheetImport with the input to the AllenExperimentsForGene service





- When we run the workflow, we can see that there are four values for the results (as there were 4 gene names that we read from the spreadsheet).
- Taverna implicitly iterated over these 4 input values and processed them.

Cli	ck in tree to vi	ew values
▼	🚞 List with 4 val	ues
	Value 1	
	Value 2	
	🖹 Value 3	
	Value 4	



Exercise 3: Saving workflow results

- Taverna allows you to save results in different formats and also allows you to save intermediate workflow results (which is very useful when you run a large workflow)
- You can save all result values:

	Workflow run data saver	
	Select the workflow input and output ports to save the associated data	
iishe	Workflow outputs:	Show workflow returns
	Value type Value type	Save value

• Taverna allows you to save values in a variety of formats



 In order to save intermediate values, in the results tab select the part of the workflow which you want to save the values for, then in the results window you should see these values and you will be able to save them

/gbif:help>

Value 4







Summary

- You can now
 - Create workflows from a variety of services
 - Connect services together
 - Run workflows
 - Use input values from different sources
 - Save workflows
 - Save results