Taverna Components

Aleksandra Pawlik
myGrid Team
University of Manchester

VLIZ, 2014-10-06 / 2014-10-08
http://www.taverna.org.uk/

What is a component?

- Something that can be put into a workflow
  - Well described - what the component does
  - Behaves “well” - conforms to agreed good practice
  - Curated - someone looks after it
  - Produces and consumes data in agreed formats
  - Fails in described ways - meaningful error messages
  - Produces agreed type of provenance
- Documentation
- Example usage

Usefulness of components

- Hide complexity
- Predictable good behaviour
- Guaranteed to work together
- Can (in theory) check that data in a run conforms to the component specification

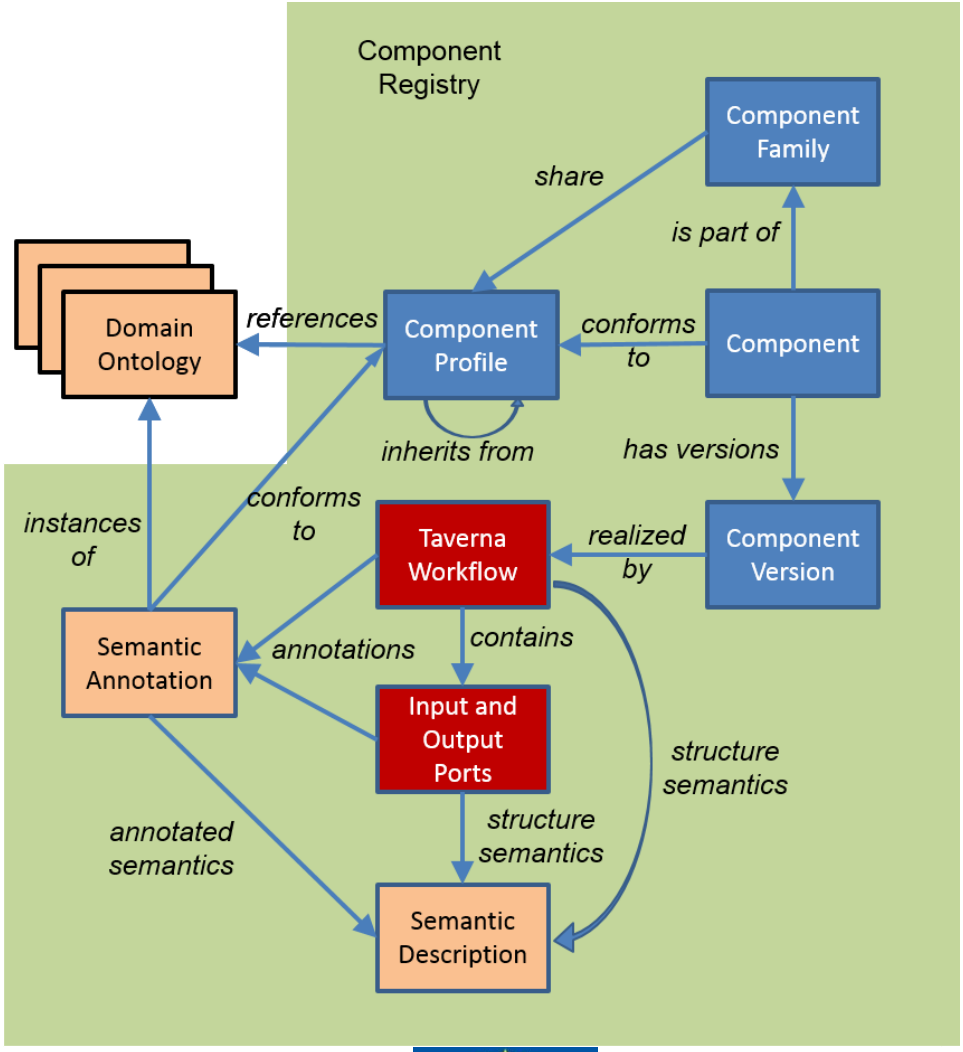
What is the agreement?

- The agreement is a condition of being in a "component family"
- Different domains, or even different uses within a domain, have different agreements
  - Astronomical data is not in the same formats as biodiversity data
  - Digital library components do not do the same tasks as biodiversity components
- Agreement is formalized as a "component profile"

Implementation

- A component family is
  - a pack on myExperiment, or
  - a directory on your local machine
- A component is defined by a workflow (in a pack) in a component family pack
- Components are versioned by the myExperiment's versioning
- Semantic annotations are stored in RDF as part of the workflow definition
- Collated semantics, including workflow structure, are combined on myExperiment.

Implementation



Component pack

- Contains:
  - Workflow ‘realizing’ the component
  - Example data
  - Documentation
  - Dependency specification

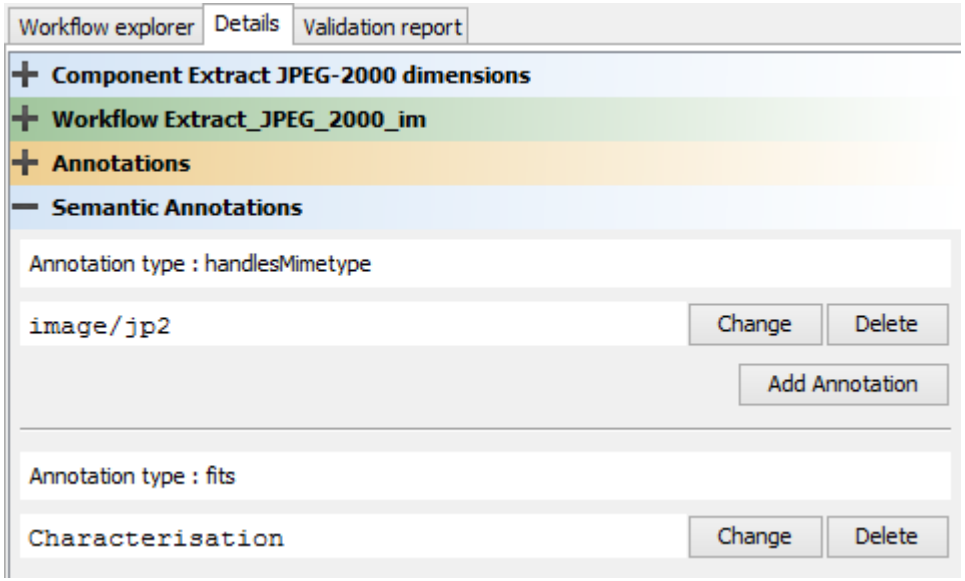
Component use

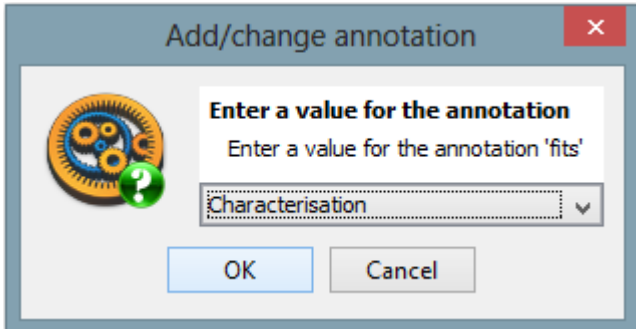
- A component family is shown in the service panel of Taverna workbench
- Components can be included within a Taverna workflow
- Components are **not** simply the same as nested workflows
  - You could think of them as nested workflows that obey a set of rules and where you cannot see what is nested (and should not care)

Component creation

- Components are created by annotating a workflow
  - Choice of a component family and so profile
  - Semantic annotation from the specified ontologies
  - Validation against the profile
  - Component saved into the component family
- Can annotate:
  - Workflow
  - Input/Output ports
  - Services inside workflow
- Extensions to myExperiment for
  - Pack snapshots
  - Semantic collation
  - Semantic searching

Semantic annotation





Turtle annotations

```
<>
      <http://purl.org/DP/components#fits>
              <http://purl.org/DP/components#Characterisation> ;
      <http://purl.org/DP/components#handlesMimetype>
              "image/jp2"^^<http://www.w3.org/2001/XMLSchema#string> .
```

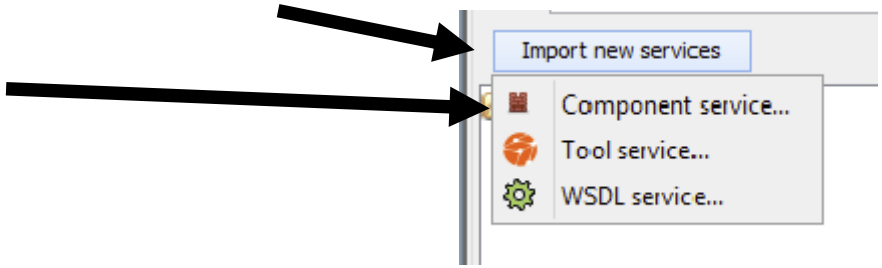
Effect on workflows

- Use of components will allow
  - Component developers to work on the component
  - Component users to upgrade (or revert) the component versions
  - A workflow to remain ‘unchanged’ (if the component interfaces remain the same)
    - Powerful and dangerous
  - Proxies for components (re-run and re-play)

- Components are “black boxes” in the workflow and workflow runs

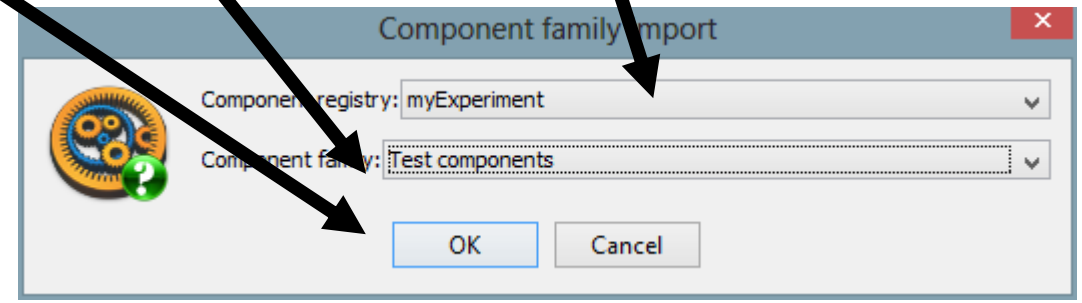
Importing a component family

- **Components** are grouped into **component families**
- **Component families** are held in a **component registry**
- myExperiment is a component registry
- You can import a component family into the **Service Panel**
- Click **Import new services** and then
- **Component service…**



Selecting a component family

- In the dialog
- Select *myExperiment* component registry, and
- *Test components* family
- Click **OK**



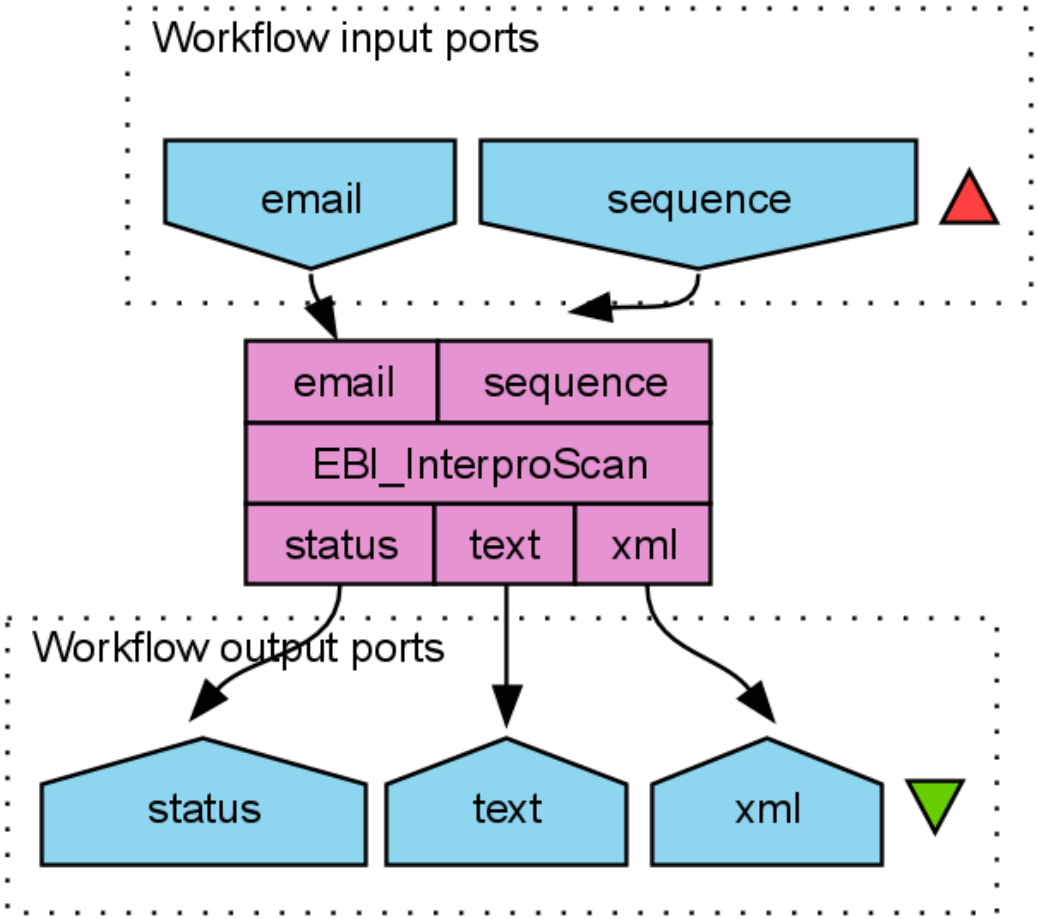
Added component family

- In the **Service panel** you can now expand and see the *Test components* family

Adding a component to a workflow

- Create a new workflow
- Add the EBI_InterproScan component into the workflow
- Create input and output workflow ports and connect them to the ports of the component

EBI InterproScan component



Running the workflow

- You can now run the workflow
- The value for the sequence should be something like:

>sp|Q9BTV4|TMM43_HUMAN Transmembrane protein 43 OS=Homo sapiens GN=TMEM43 PE=1 SV=1

MAANYSSTSTRREHVKVKTSSQPGFLERLSETSGGMFVGLMAFLLSFYLIFTNEGRALKT

ATSLAEGLSLVVSPDSIHSVAPENEGRLVHIIGALRTSKLLSDPNYGVHLPAVKLRRHVE

MYQWVETEESREYTEDGQVKKETRYSYNTEWRSEIINSKNFDREIGHKNPSAMAVESFMA

TAPFVQIGRFFLSSGLIDKVDNFKSLSLSKLEDPHVDIIRRGDFFYHSENPKYPEVGDLR

VSFSYAGLSGDDPDLGPAHVVTVIARQRGDQLVPFSTKSGDTLLLLHHGDFSAEEVFHRE

LRSNSMKTWGLRAAGWMAMFMGLNLMTRILYTLVDWFPVFRDLVNIGLKAFAFCVATSLT

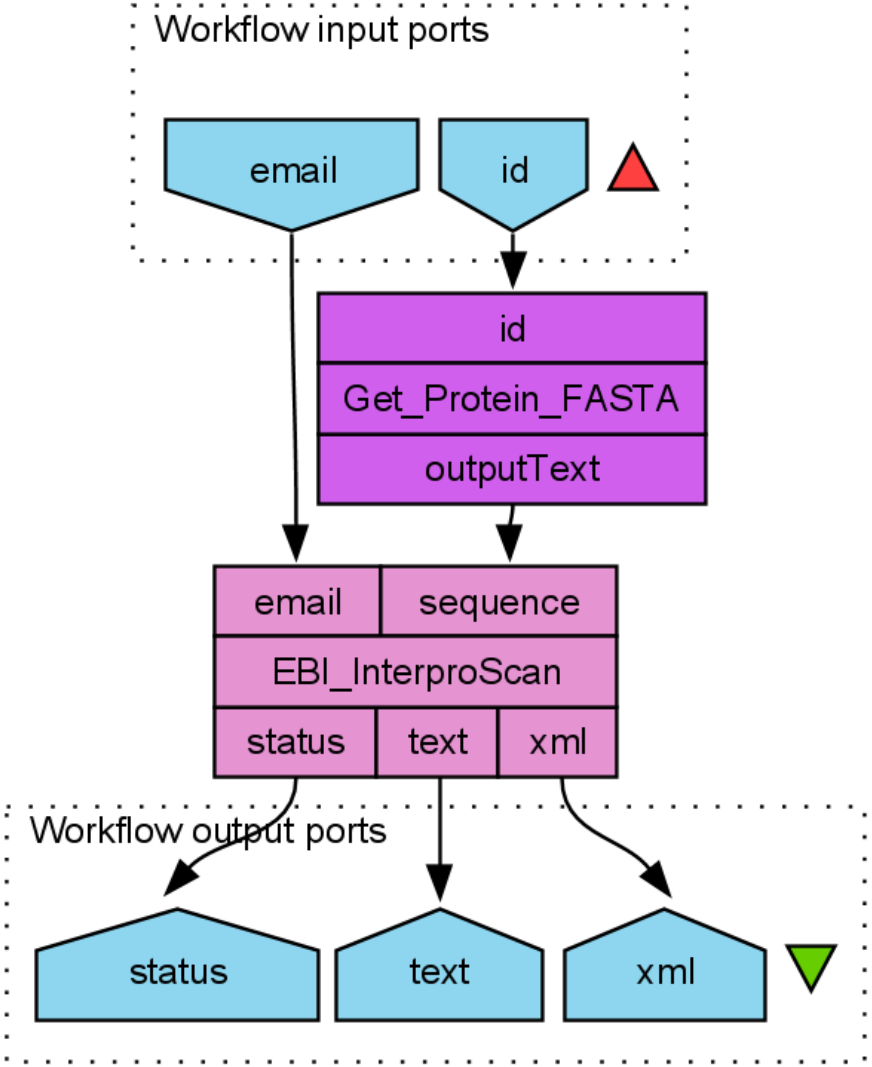
LLTVAAGWLFYRPLWALLIAGLALVPILVARTRVPAKKLE

Connecting components

- The workflow just contains the single service, we need to connect the component with other services
- In the **Design view**, delete the *sequence* workflow input port
  - Right click and select **Delete workflow input port**
- Add **Local Services** -> **ncbi** -> **Get Protein FASTA** to the workflow
- Connect the *outputText* of *Get Protein FASTA* to the *sequence* port of the *EBI_InterproScan*
- Connect the *id* port of *Get Protein FASTA* to a workflow input port

Connected component

Your workflow should now look like:



Running the workflow - 2

- Run the workflow again
- You can use Q9BTV4 as the value for *id*

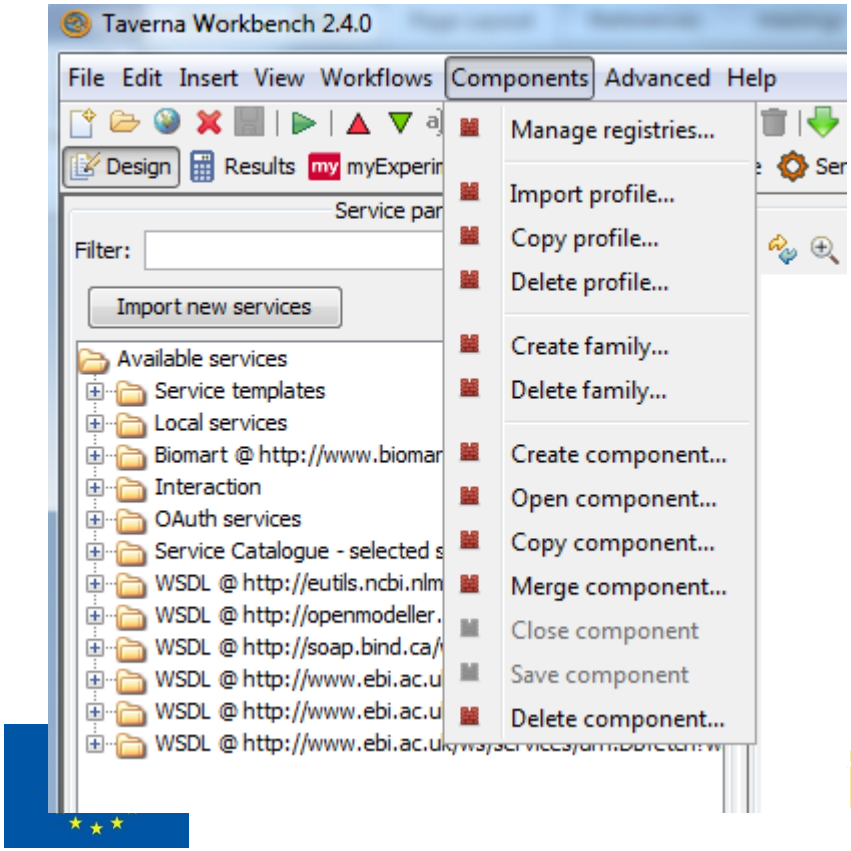
Is it really the complex workflow?

- In the **Results view** you can click on **Progress report**
- Expand *EBI_InterproScan*
- You can see all the services “hidden” inside the component

Workflow1	Finished
EBI_InterproScan	Finished
getTextResult	Finished
getTextResult_input	Finished
getTextResult_output	Finished
getXmlResult	Finished
getXmlResult_input	Finished
getXmlResult_output	Finished
input	Finished
run	Finished
run_input	Finished
run_output	Finished
Status	Finished
getStatus	Finished
getStatus_input	Finished
getStatus_output	Finished
tsv - tsv	Finished
xml - xml	Finished
Get_Protein_FASTA	Finished

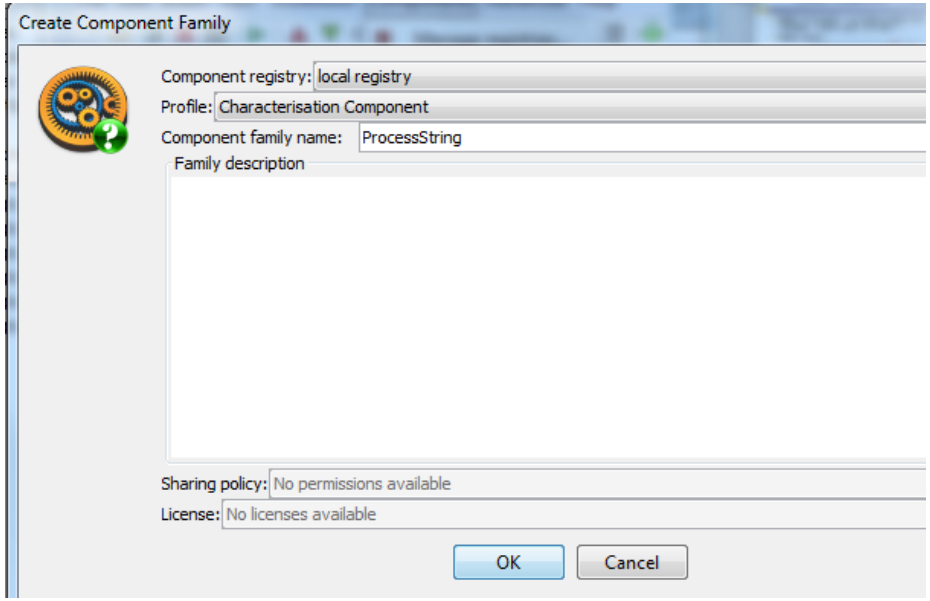
Taverna Components in practice

- The menu has a “Components” option
- Select “Create family”



Taverna Components in practice

- In the pop-up window set the registry to local
- Select a Profile (or see next slide if no profile available)
- Enter the family name ("ProcessString")



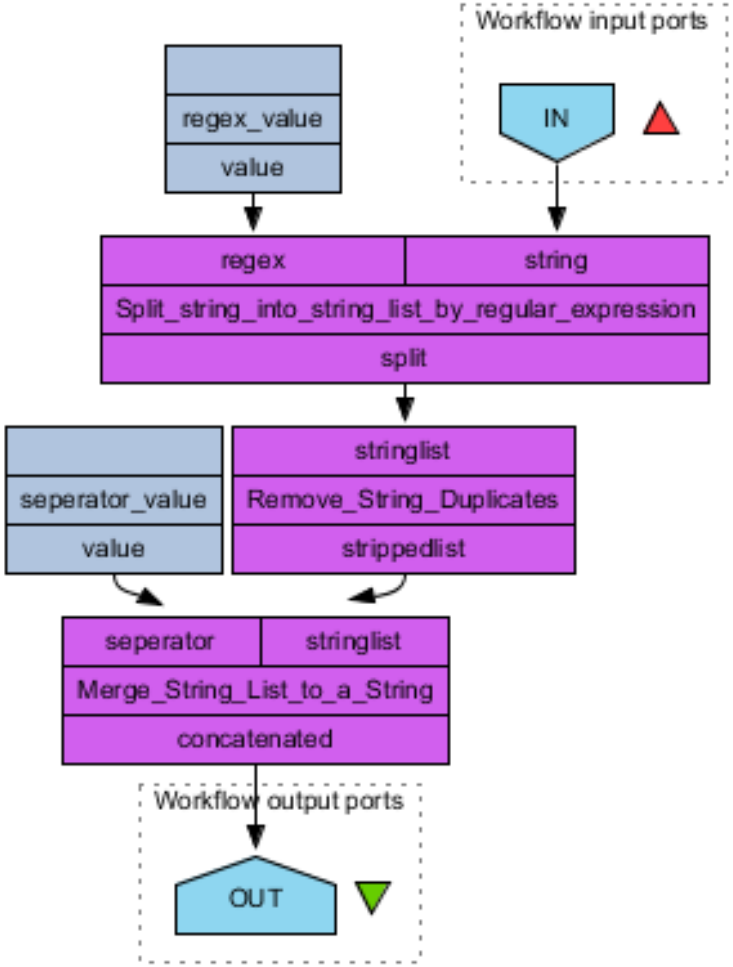
Adding a Profile (if required)

- Select Components/Import Profile (from the menu)
- Set Profile URL to:
  - http://www.myexperiment.org/files/1027/versions/2/download/EmptyProfile.xml
- Press OK

Taverna Components in practice

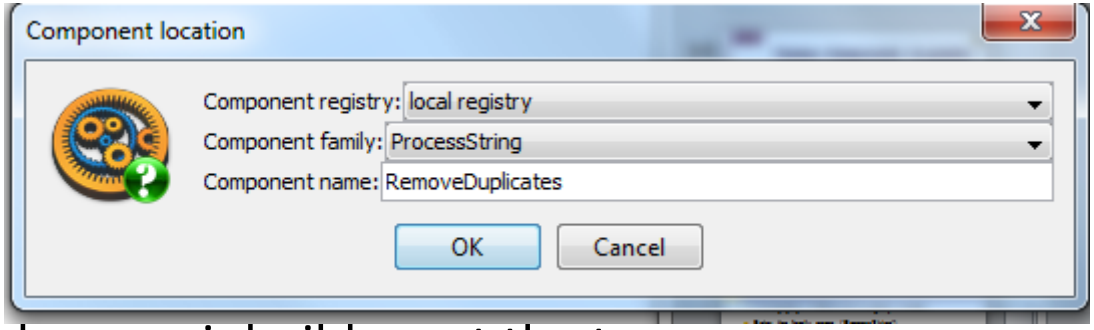
- Add a local service “Split string into string list by regular expression” (from ‘text’)
- Add the input port and set the regular expression to space
- Add a local service “Remove string duplicates” (from ‘list’)
- Connect the output from “Split string into string list by regular expression” with the input of “Remove string duplicates”
- Add a local service “Merge String List to a String” and connect its input with the “Remove string duplicates” output and set the separator to be a space

Taverna Components in practice

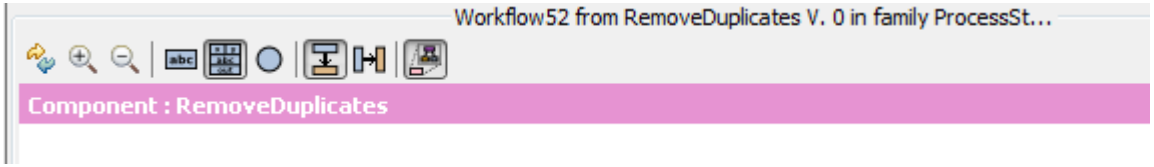


Taverna Components in practice

- Select “Create component” from the “Components” menu
- Provide a name for the component (Remove duplicates)



- You should see a pink ribbon at the top



- Save the component. You will see a warning message – it pops up because the component is not annotated. We can annotate it in the component details.

Using your Component

- Close any open workflows
- Add the component(s) to the service panel
  - Hint: Import Service/ Component Family
- Component registry: Local registry
- Component family: ProcessString
- Add the component to the workflow
  - Hint: Available services/ Components …
- Add input and output ports
- Run