PhUSE CSS

Linked Data for Clinical Trials

An Interactive Hands-on Workshop

EXERCISES

Version 3.0

04 March 2018

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# Introduction

Instructions in this document are specific to the PhUSE cloud server environment, Graph Editor application and workshop methods. The exercises represent one of many possible approaches to the material and make no claim to be best or recommended method. The instructor will complete the exercises during the session, along with the attendees.

Your feedback is welcomed and encouraged. Please send your comments to: **tim.williams@PhUSE.eu**

## Materials

* Laptop with Remote Desktop capability
* Printed copies of the following will be supplied by the instructor:
  + Exercises (this document)
  + Info Sheet
  + Graph Editor Reference

## Symbols and Conventions

Symbols provide important information:

|  |  |
| --- | --- |
|  | Stop and wait. Do not proceed to the next section until instructed. |
| **!** | Cautions and warnings. Failure to follow these steps may lead to unanticipated results and problems. |
|  | The instructor presents important material at this point. |
| IdeaIcon_clean_20mm | Helpful tips and advice. |
| Image result for information icon | Additional information. |

# Server Login

Login to the cloud server using Remote Desktop. Instructions assume Windows 10 operating system.

1. In the search box on the taskbar on your laptop, type **remote desk,** then select **Remote Desktop Connection** from the Programs section.﻿
2. Click **Show Options** if needed to show the fields for **Computer:** and **User name:**

The instructor will provide the password and an IP Address for the Computer: field.

**Computer:** \_\_\_\_\_\_\_\_\_\_\_\_\_\_

(See Info Sheet)

**User name:** phuseldw

**Password:** \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

(Provided by Instructor)

1. Entering values in the **Computer:** and **User name:** fields, then click **Connect**.
2. When prompted, enter the password supplied by the instructor and click **OK**.

|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor.  Presentation follows |  |

# Exercises

# Create a Graph in the Graph Editor

# Open the Graph Editor

On the cloud server:

1. Open Google Chrome.
2. Click on "GraphEditor" on the shortcuts bar. 
3. The Graph Editor opens and shows two IRI nodes: One for **Drug1** and one for the drug's name, **Serum114.**



Ask for assistance if you do not see these nodes.

# Add a Clinical Trial, Trial Phase, and Treatment Arms

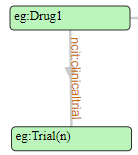
|  |  |
| --- | --- |
| **!** | When you see values like Trial**(n)**, Phase**(n)**, Treatment**(n)**, etc. you must change your graph to values you find in the Info Sheet or create on your own. The values used in your graph become : Trial**1**, Phase**3**, Treatment**7-1**, etc. |

Create a node that represents unique clinical **Trial** conducted for **Drug1** and the Treatments for that trial. Reference the Info Sheet for values where needed.

1. Create a **Trial** node with these values:

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | *Info Sheet: x.x: [Trial1]* | Image result for information icon*See Info Sheet for value* |
| **Type:** | IRI |  |



1. Create the relation ***from*** **Drug1** ***to*** the **Trial** node:

Link values:

|  |  |
| --- | --- |
| **Prefix:** | ncit |
| **Label:** | clinicaltrial |

1. Create a Trial **Phase** node. You may choose any of these phases: **Phase2**, **Phase3**, **Phase4.**

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | ncit |  |
| **Label:** | *Choose a value:* | Image result for information icon*You choose a value for phase:* **Phase2, Phase3, Phase4**  *NO SPACE in the name!* |
| **Type:** | IRI |  |

1. Create the link ***from*** the **Trial** ***to*** the Trial **Phase**.

Link values:

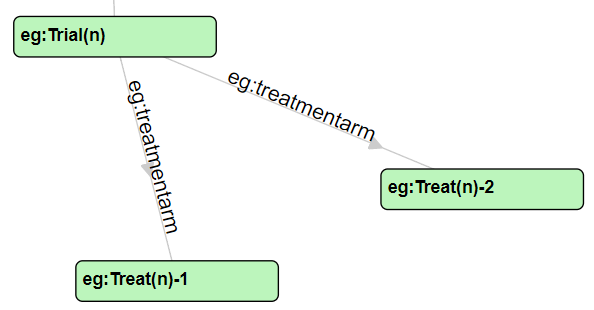
|  |  |
| --- | --- |
| **Prefix:** | ncit |
| **Label:** | phase |

1. Create two **Treatment** nodes for the **Trial**.

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | *Info Sheet: x.x, x.x [Treat1-1,Treat1-2]* | Image result for information icon*See Info Sheet for values.* |
| **Type:** | IRI |  |

Ensure you have two treatment nodes in your graph.



1. Create the relations ***from*** the **Trial** ***to*** the two **Treat**ment nodes.

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | treatmentarm | Image result for information icon*Label is all lowercase.* |

Link values:

There should now be one treatmentarm link to each of the **treatment** nodes.

1. Create two "treatment type" nodes to represent **Placebo** and **Active** treatments

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | Placebo |  |
| **Type:** | IRI |  |

Node values:

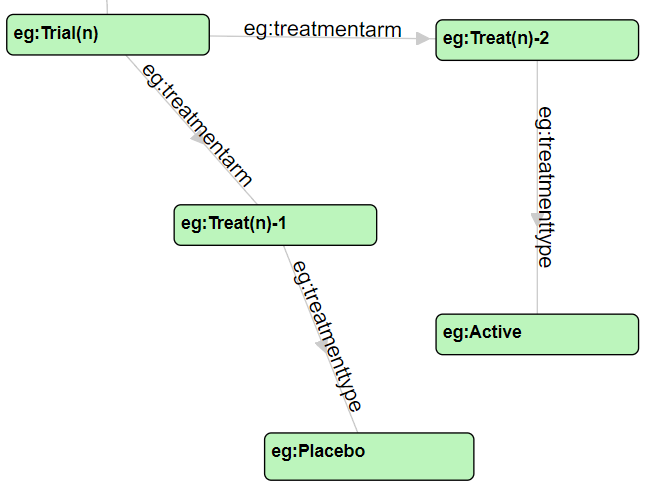
|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | Active |  |
| **Type:** | IRI |  |

1. Now join each **Treat**ment node (created in step x) to one of the Treatment Type nodes using the following relationship. It does not matter which is the A**ctive** or P**lacebo**. You will create two edges:

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | treatmenttype | Image result for information icon*Label is all lowercase.* |

The **Trial** and **Treat**ment portion of your graph should look similar to:



|  |  |
| --- | --- |
| IdeaIcon_clean_20mm | Click  to create a copy in case anything goes wrong in the next steps. |

# Add Persons and Treatments

1. Add three **Person** nodes to the graph:

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | *Info Sheet: x.x, x.x , x.x [Person11, Person12, Person13]* | Image result for information icon*See Info Sheet for values.* |
| **Type:** | IRI |  |

1. For two of the **Person** Nodes: Create ***enrolledin*** relations ***from*** the **Person** ***to*** the **Trial** node.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | enrolledin | Image result for information icon*Label is all lowercase.* |

1. For the remaining **Person** node: Create a ***primaryinvestigator*** link ***from*** the **Person** node ***to*** the **Trial** node.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | primaryinvestigator | Image result for information icon*Label is all lowercase.* |

1. Assign one of the two **Person** nodes ***enrolledin*** the Trial to one of the **Treat**ments by creating the ***treatment*** link ***from*** that **Person** ***to*** the **Treat**ment.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | treatment | Image result for information icon*Label is all lowercase.* |

1. Repeat for the second person node ***enrolledin*** the Trial by creating a link ***from*** the **Person** node ***to*** the other **Treat**ment.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | treatment | Image result for information icon*Label is all lowercase.* |

Now both **Person**s ***enrolledin*** the **Trial** are assigned to **Treat**ments. The **Person** with ***primaryinvestigator*** relationship is not assigned to a **Treat**ment.

# Add Gender to Persons

1. Create a node for **Male** and an node for **Female .**

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | Male |  |
| **Type:** | IRI |  |

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | Female |  |
| **Type:** | IRI |  |

2. Create links ***from***all 3 **Person** nodes ***to*** a Gender value using the ***gender*** relation.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg |  |
| **Label:** | gender | Image result for information icon*Label is all lowercase.* |

|  |  |
| --- | --- |
| IdeaIcon_clean_20mm | Click  to save a copy of your graph. |

# Demographics for Person Nodes

A. Create a **Name** for each **Person** in the graph:

1. Create **Name** nodes as strings:

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** |  | Image result for information iconPrefix is not applicable to literals. You may ignore this field. |
| **Label:** | *<Any name you want>* |  |
| **Type:** | STRING |  |

2. Link ***from*** a **Person** ***to*** a **Name** use the ***name*** relation.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | schema | Image result for information icon Many other prefixes could be used here. |
| **Label:** | name |  |

B. Add an **Age** (in years) for each **Person.**

1. Create **Age** nodes as INT (integers):

Node values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** |  | Image result for information iconPrefix is not applicable to literals. |
| **Label:** | *<Any age integer value you want>* |  |
| **Type:** | INT |  |

2. Link ***from***a **Person** ***to*** an age using the ***age*** relation.

Link values:

|  |  |  |
| --- | --- | --- |
| **Prefix:** | eg | Image result for information icon eg is used because age calculation may be specific to this graph. |
| **Label:** | age |  |

|  |  |
| --- | --- |
| IdeaIcon_clean_20mm | Click  to save a copy of your graph. |

**Optional Activity**

Time permitting, you may create these additional nodes while you wait for the class to catch up. Do not add too many nodes or your whiteboard may become difficult to read.

C. Add additional Person nodes and assign them to a Treatment.

D. Add additional treatments, or add details to the existing treatments.

|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor. |  |

# Export to TTL

1. **As for the instructor orassistant to review your graph prior to taking the next steps. Click**  **if you make any changes.**
2. Click on  to export the graph to TTL format.
3. The graph will be saved to your downloads folder as **WhiteBoardTriples.TTL :**

**C:\Users\phuseldw\downloads\WhiteBoardTriples.TTL**

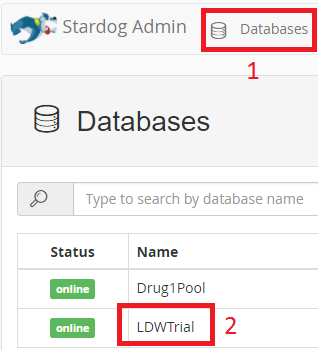
|  |  |
| --- | --- |
| **!** | Leave the graph open in Chrome. You will refer to it in the next section when creating queries. Ask for assistance if you accidentally close or refresh the Graph Editor window. |

1. Use Windows explorer to navigate to the TTL file.
2. Double click on the .TTL file to open it.
3. Follow along with the instructor's explanation of the TTL file content.
4. Find the various ***nodes*** and ***links*** you created in your graph.

|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor. |  |

# Upload to Triplestore

1. Open a new window in Google Chrome, keeping your graph editor window open.
2. Click the Stardog shortcut on the bookmarks bar.



1. Click "Databases" on the top menu
2. Double-click the row for **LDWTrial.**
3. In the upper right, click 



1. Select **Data | Add** from the Stardog menu:
2. Click **Browse** and navigate to the TTL file you created from the GraphEditor and load it into Stardog.

C:\Users\phuseldw\Downloads\**WhiteBoardTriples.TTL**

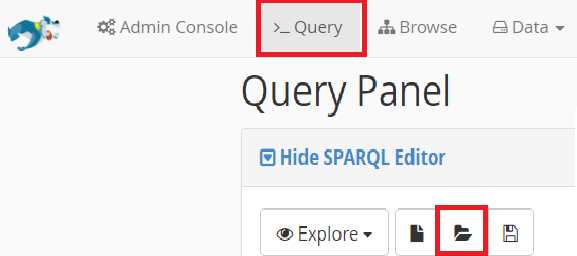
|  |  |
| --- | --- |
| **!** | Multiple copies of the TTL file will be present if you exported to TTL more than one time.: WhiteBoardTriples (1).TTL, WhiteBoardTriples (2).TTL, etc. Choose the most recent file with the largest (n) number in the name. |

1. Click **Upload**.
2. You should see the message: Success! Data added successfully.

# Query your graph

# Show all triples

Query the graph to find all Subject-Predicate-Object relations in your graph.

1. If the "Query Panel" is not displayed, click on the >\_Query menu item at the top of the Stardog display.
2. Select the Open Folder icon  in the Query Panel.
3. Navigate to the file C:\LinkedDataWorkshop\**scripts\SPARQL\100-AllTriples .rq** . Double-click the file to load it into the query window.
4. With the query loaded in to the window, click the  button. Scroll down to review the results.
5. Compare this view to what you expected after viewing the TTL file.

# How many people *enrolledin* the trial?

You graph only contains the information for the one trial, you can count the number of *enrolledin* relationships.

1. Load the SPARQL query **101-CountEnrolledIn.rq**.
2. Examine the query while the instructor explains how it relates to your graph.
3. Execute the query.
4. Note how the primary investigator is not included in the count.

# Find the names of people who *enrolledin* your trial.

In this example you want to select the name of the Persons enrolled in the trial.

1. The result should be the Person's name:

SELECT ?name

1. Your query must first identify Person nodes that have the ***enrolledin*** relation:

?person eg:enrolledin ?trial ;

1. Then follow from that Person node using the name relation to find their name.



?person eg:enrolledin ?trial ;

schema:name ?name .

1. Try writing and executing the query in the query window using the code snippets above.
2. If you have trouble, load and execute the query: **102-NameEnrolledIn.rq**

# List the names of the people in each treatment type.

Adapt your query in the previous exercise to create a list of the people within each type of treatment.

1. Change your SELECT statement to select treatment type and name variables. Example:

SELECT ?treattype ?name

1. Change your WHERE statement to include the path from ?person to ?treatment through the ***treatment*** relation, then follow ***from*** the ?treatment ***to*** the treatment type by following the ***treatmenttyp***e relation.

?person eg:enrolledin ?trial ;

schema:name ?name ;

eg:treatment ?treatment.

?treatment eg:treatmenttype ?treattype;

1. Sort the result by treatment type using ORDER BY

ORDER BY ?treattype

SOLUTION: **103-NamesInTreatmentType.rq**

|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor.  Presentation on Ontologies and Reasoning |  |

# Ontology

In this section you will add an ontology to the data and use it for reasoning.

# Review the Ontology

1. Double-click on the file C:\LinkedDataWorkshop\data\**TrialOntology.TTL** to open into a text editor.
2. Follow along with the instructor's explanation of the file.

# Add the Ontology to the LDWTrial database

1. Select Data | Add from the Stardog menu.
2. Click **Browse** and select the file:

C:\LinkedDataWorkshop\**data\TrialOnotology.TTL**

Click **Upload**.

1. You should see the message: **Success! Data added successfully.**

# Explore the data



1. Ensure reasoning is turned OFF.
2. Select **Explore | Class Hierarchy**
3. A SPARQL query appears in the window.
4. **Execute** the query and view the results. Only rdfs:Class and rdfds:Property is returned.



1. Turn on the reasoner by clicking the **Reasoning** button.
2. **Execute** the query again and view the results.

|  |  |
| --- | --- |
|  | The instructor explains the source of these new triples. |

# Query with Reasoning

Reasoning allows you to query using new types (classes) of nodes and inferred relationships.

# Find the names of HumanStudySubjects *enrolledin* your trial.

Your original data contained no definition of a HumanStudySubject.

1. Review the ontology file for how a HumanStudySubject is *inferred* using the ontology.

|  |  |
| --- | --- |
| IdeaIcon_clean_20mm | In SPARQL the predicate rdf:type can be shorted to a and interpreted as "is a".  Example:  You read: eg:Person11 rdf:type eg:HumanStudySubject  as: "Person11 is a HumanStudySubject." |

Instead of querying on the enrolledin predicate, as in:

?person eg:enrolledin ?trial ;

You can now query using the *inferred* entity eg:HumanStudySubject.

?person a eg:HumanStudySubject;

1. Modify your original query in Section X.X (**102-NameEnrolledIn.rq ) to use** eg:HumanStudySubject.
2. Ensure Reasoning is turned on, then execute the query.

Solution: **202-NameHumanStudySubject.rq**

Bonus Question: How would you modify the query to select all Investigators in the trial?

Hint: How is Investigator defined in the ontology file?

Solution: **203-NameInvestigator.rq**

# Write a reasoner-based query to find all People associated with the trial.

Your query should have a one-line statement the uses the superclass for both HumanStudySubjects and Investigators using the superclass of these two classes.

CAUTION: The superclass prefix is not "eg:" because that class is borrowed from another ontology!

Solution: 204-NamesAllPeople.rq

|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor.  Presentation on Merging Data |  |

# Merging data from all trials

|  |  |
| --- | --- |
|  | Instructor creates a single database of all merged trials, live demo. When the pool is ready from the instructor you will load a copy into your local Drug1Pool database. |

# Obtain a copy of the pooled data.

1. Click on Admin Console at the top of the Stardog application. 



1. Click on **Drug1Pool** in the Databases panel.
2. In the upper right, click 
3. Open the query **300-GetDataPool.rq** into the query window an execute it. A blue progress line will display briefly at the top of the application while the query is executing.
4. After the query has completed, execute the query **301-PoolTripleCount.rq**. Note the number of triples and compare them to the number provided by the instructor to ensure you have the correct data.

# List Drug1 trials by phase.

1. Load the query **302-TrialsByPhase.rq** . Examine the query to see how it follows the graph model.
2. Execute the query and locate your trial in the results.

# How many HumanStudySubjects participated in Drug1 trials?

1. Ensure the Reasoner is turned on.
2. Load the query **303-Drug1CountHSS.rq** and examine the query.
3. Execute the query.

BONUS : Alter the query to count **all people** involved in Drug1 Trials (not just HumanStudySubjects).

HINT: What is the superclass of HumanStudySubject?

# What is the gender breakdown for HumanStudySubjects across all Drug1 trials?

[TO HERE. FIXING DATA ERROR]

# Identify patients that participated in multiple trials.

Bonus2: List names of all people involved in Drug1 trials by trial and by role.

[instructions to sign out from server]

Congratulations! You've made to the

---- END OF THE EXERCISES ----

|  |  |  |
| --- | --- | --- |
|  | Stop here and wait for the instructor.  Presentation follows |  |

# Appendix 1: Course Resources

* [Introduction to Semantic Web](http://www.cambridgesemantics.com/semantic-university/introduction-semantic-web)

http://www.cambridgesemantics.com/semantic-university/introduction-semantic-web

* [What is Linked Data?](http://www.cambridgesemantics.com/semantic-university/what-linked-data)

http://www.cambridgesemantics.com/semantic-university/what-linked-data

* [Introduction to Linked data](http://www.cambridgesemantics.com/semantic-university/introduction-linked-data)

http://www.cambridgesemantics.com/semantic-university/introduction-linked-data

* [Learning SPARQL](http://www.learningsparql.com/)

http://www.learningsparql.com/

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[Hands-on Workshop Github Repository](https://github.com/phuse-org/LinkedDataWorkshop/tree/master/Annual2017-EU)

Course content is available at:

https://github.com/phuse-org/LinkedDataWorkshop/tree/master/CSS2018