

## Techie Table

**Duration:** 3 hours

### **Description of Activity:**

The discussion will be organized in two parts: In the first part we are going to show how a developer can consume OpenTox web services from inside a Java application using some tools of ours. This will include some A&A (Authorization and Authentication) also. Using web clients and parsers, the participants will download and parse OpenTox resources such as compounds, features, datasets and models and inspect them from within their Java application. Exercises will include parsing of datasets and conversion into weka data objects (Instances), training of various models using NTUA, TUM and AMBIT algorithms (where necessary using also the A&A API). So this will familiarize the participants with the direct consumption of OT web services on a more advanced level than using web interfaces and a more programmatic way than using plain curl. This will take about 45 minutes including discussion/questions.

In the second part, we will have the audience building an OpenTox web service with some guidance. A clustering algorithm will be deployed for the sake of getting in touch with web services and having a better insight into the OpenTox API. First we will study the requirements of the OT API and will formulate hypothetical curl commands for how a request would look like (In a top-down approach). Then we will proceed formulating an RDF representation of the algorithm discussing at the same time about the structure of such a document and the information that should be found therein. Jena will be used as an RDF editor/parser, which will be quite useful to developers that want to get involved into any contemporary project (web semantics etc). We will not get into much detail as far as the storing of models is concerned but briefly we'll present the underlying database tables structure. Weka will be used to materialize the XMeans algorithm. The whole effort will boil down to just about 500 lines of source code including the use of various Java libraries such as Restlet, Weka and Jena. This will take about 75' and the rest of the time we will discuss about various challenges a developer can take.

### **Experience Expected:**

A moderate acquaintance with Java is needed to join the table. The participant should know how to use some IDE of his/her preference and know how to create a Java application and load libraries. Some acquaintance with HTTP and web services is also needed.

### **Preparation before joining the table:**

We would suggest that participants examine the OpenTox API to gain a better insight into the OpenTox services. The API is available from the OpenTox web site at <http://opentox.org/dev/apis/api-1.1>.

Before joining the table, the participant should have installed the following on his machine:

1. An IDE. I would suggest [Netbeans](#) (version >6.8)
2. Java, version 1.6. On a Linux machine, type 'sudo apt-get install sun-java6-jre' and 'sun-java6-jdk'. For other operating systems, you can download and install Java from <http://www.java.com/en/download/manual.jsp> . Mac OSX supports its own version of Java.
3. Java DB (Apache Derby) version 10.6.1. Download the jars from <http://wiki.apache.org/db-derby/DerbyTenSixOneRelease>. Load it in you IDE (e.g. [Netbeans](#)) as a library.

Optional applications the user might want to install:

1. Git: Download and install git from <http://git-scm.com>. Git can be also found in the Linux repositories. Install it typing 'sudo apt-get install git-core'.
2. Install cURL from <http://curl.linux-mirror.org> or simply type 'sudo apt-get install curl'
3. Download and run Protégé, an ontology editor that will let you examine the ontology used in OpenTox to describe resources such as algorithms, compounds, features etc. Protege can be found at <http://protege.stanford.edu>. Use Protégé to view the ontology at <http://opentox.org/data/documents/development/RDF%20Files/OpenToxOntology>.

The following Java libraries should be downloaded and loaded in your IDE:

1. Restlet, version 2.0 milestone 7: Download it from the URL: <http://www.restlet.org/downloads/2.0/restlet-jse-2.0m7.zip>. Read about Restlet at <http://www.restlet.org/about/introduction> and find some example applications at [http://wiki.restlet.org/docs\\_2.0/13-restlet/21-restlet/318-restlet.html](http://wiki.restlet.org/docs_2.0/13-restlet/21-restlet/318-restlet.html)
2. Xstream, version 1.3.1: Download Xstream from: <http://repository.codehaus.org/com/thoughtworks/xstream/xstream-distribution/1.3.1/xstream-distribution-1.3.1-bin.zip>.
3. Jena, version 2.6.2: Download Jena from <http://sourceforge.net/projects/jena/files/Jena/Jena-2.6.2/jena-2.6.2.zip/download>.
4. Download Reflections, version 0.9.5. from <http://code.google.com/p/reflections/downloads/list>.
5. Weka 3.6.0. can be downloaded from <http://sourceforge.net/projects/weka/files/weka-3-6/3.6.0/weka-3-6-0.zip/download>. Weka is a machine learning library for Java.
6. Download iText version 5.0.1. from <http://sourceforge.net/projects/itext/files/iText/iText5.0.1/iText-5.0.1.jar/download>. iText is a PDF editor for Java.
7. Download and examine the source code of YAQP (Yet Another QSAR Project), from <http://github.com/alphaville/yaqp-turbo>. Click on the “Download Source” button or

using *git*, type 'git clone git://github.com/alphaville/yaqp-turbo.git'

If you need help installing any of the above software or libraries, please contact Pantelis Sopasakis via email at [chvng@mail.ntua.gr](mailto:chvng@mail.ntua.gr) or reach me at MSN: [aureliacosmetics@yahoo.gr](mailto:aureliacosmetics@yahoo.gr).

#### References:

1. The OpenTox web site: <http://opentox.org>
2. Restful Web Services: [http://en.wikipedia.org/wiki/Representational\\_State\\_Transfer](http://en.wikipedia.org/wiki/Representational_State_Transfer).  
Read also this note on our web site: <http://opentox.org/dev/framework/restweb>.
3. OWL Validation Online Tool: <http://www.mygrid.org.uk/OWL/Validator>.
4. RDF Validation Online service by W3C: <http://www.w3.org/RDF/Validator/> (Also produces graphical representations of RDF documents)