INSTALLING THE GINAS, PUBLIC VERSION ON UBUNTU 16.04
USING POSTGRESQL 10 AS DATABASE

Ginas Monthly Meeting
Feb 7th, 2017
Alex Welsch

A. Slides
B. Details with CLI commands below
A. Slides

Get the program and sample data

https://tripod.nih.gov/ginas/#/gsrs/
Unzip the downloads

<table>
<thead>
<tr>
<th>Name</th>
<th>Size</th>
<th>Type</th>
<th>Modified</th>
</tr>
</thead>
<tbody>
<tr>
<td>bin</td>
<td>3 items</td>
<td>Folder</td>
<td>Oct 11 2017</td>
</tr>
<tr>
<td>conf</td>
<td>13 items</td>
<td>Folder</td>
<td>Feb 6</td>
</tr>
<tr>
<td>ginas.idx</td>
<td>6 items</td>
<td>Folder</td>
<td>Oct 11 2017</td>
</tr>
<tr>
<td>lib</td>
<td>167 items</td>
<td>Folder</td>
<td>Oct 11 2017</td>
</tr>
<tr>
<td>logs</td>
<td>5 items</td>
<td>Folder</td>
<td>00:01</td>
</tr>
<tr>
<td>share</td>
<td>1 item</td>
<td>Folder</td>
<td>Oct 11 2017</td>
</tr>
<tr>
<td>access-log-2018-02-06.gz</td>
<td>2.8 kB</td>
<td>Archive</td>
<td>00:01</td>
</tr>
<tr>
<td>application-log-2018-02-06.gz</td>
<td>35.3 kB</td>
<td>Archive</td>
<td>00:00</td>
</tr>
<tr>
<td>RUNNING_PID</td>
<td>4 bytes</td>
<td>Text</td>
<td>Feb 6</td>
</tr>
</tbody>
</table>
Locate "ginas.conf"
Edit "ginas.conf"

```
348 # db.default.url="jdbc:h2:~/{ix.home}/h2/ginas;MVCC=true"
349 # db.default.user=sa
350 # db.default.password=""
351 # db.default.maximumPoolSize = 50
352 #END H2 example
353 ##########################
354
355 # evolutionplugin=disabled
356
357 # This is for testing
358 # ebean.default2="ix.test.modelsb."#
359 ##########################
360 #H2 example
361 # db.default2.driver=org.h2.Driver
362 # db.default2.url="jdbc:h2:~/{ix.home}/h2/ginas;MVCC=true"
363 # db.default2.user=sa
364 # db.default2.password=""
365 #END H2 example
366 ##########################
367
368 ##########################
369 # postGreSQL example
370 # db.default.driver="org.postgresql.Driver"
371 # db.default.url="jdbc:postgresql://localhost:5432/ginas_db1"
372 # db.default.user="ginas_usr1"
373 # db.default.password="hello5"
374 #END postGreSQL example
375 ##########################
376
377 # You can specify the path to an additional mapping file to make
378 # certain keys resolve as if they were other keys (e.g. old codes)
379
380 # The expected file format is a header-less 2-column tab-delimited
381 # file. The first column is the key you want to map, and the second
382 # column is the key you want to map to. This will only be used during
383 # url resolving, and only when there are no matches with the standard
384 # ways that keys are resolved (using database lookups)
385
386 # ix.ginas.mapping.synonymsFile="/olduuldmapping.txt"
```
About "apt-get" (installing a package silly example)

```
welscha@kale:~$ sudo apt-get install cowsay
Reading package lists... Done
Building dependency tree
Reading state information... Done
The following packages were automatically installed and are no longer required:
  linux-headers-4.10.0-28 linux-headers-4.10.0-28-generic
  linux-headers-4.10.0-40 linux-headers-4.10.0-40-generic
  linux-image-4.10.0-28-generic linux-image-4.10.0-40-generic
  linux-image-extra-4.10.0-40-generic
Use 'sudo apt autoremove' to remove them.
The following additional packages will be installed:
  cowsay-off
Suggested packages:
  filters
The following NEW packages will be installed:
  cowsay cowsay-off
0 upgraded, 2 newly installed, 0 to remove and 86 not upgraded.
Need to get 0 B/21.7 kB of archives.
After this operation, 112 kB of additional disk space will be used.
Do you want to continue? [Y/n] Y
Selecting previously unselected package cowsay.
(Reading database ... 291230 files and directories currently installed.)
Preparing to unpack .../cowsay 3.03+dfsg1-15_all.deb ...
Unpacking cowsay (3.03+dfsg1-15) ...
Selecting previously unselected package cowsay-off.
Preparing to unpack .../cowsay-off 3.03+dfsg1-15_all.deb ...
Unpacking cowsay-off (3.03+dfsg1-15) ...
Processing triggers for man-db (2.7.5-1) ...
Setting up cowsay (3.03+dfsg1-15) ...
Setting up cowsay-off (3.03+dfsg1-15) ...
welscha@kale:~$
```
welscha@kale:~$ echo "Got Alfalfa?" | cowsay

< Got Alfalfa? >

\^
\ /\)
 \   \/
  \--
     \|```
Install postgres (more complicated but same idea)

```bash
myuser%> cd
myuser%> mkdir temp-pg
myuser%> cd temp-pg
myuser%> wget -q https://www.postgresql.org/media/keys/ACCC4CF8.asc -O - | sudo apt-key add -
myuser%> sudo sh -c "echo "deb http://apt.postgresql.org/pub/repos/apt/ `lsb_release -cs`-pgdg main" >> /etc/apt/sources.list.d/pgdg.list"
myuser%> sudo apt-get update
myuser%> sudo apt-get upgrade
myuser%> sudo apt-get install postgresql postgresql-contrib
myuser%> cd
```
Creating a postgres user and db

```bash
postgres=# create user ginas_usr3 with password 'hello5';
CREATE ROLE
postgres=# create database ginas_db3;
CREATE DATABASE
postgres=# grant all privileges on database ginas_db3 to ginas_usr3;
GRANT
postgres=#
```
Run ginas!
Import the sample data

Login using admin/admin as credentials; then click on Admin > Data Management
Browse substances

LIATERMIN

Names:
- LIATERMIN
- METHIONYL NEUROTROPHIC FACTOR (HUMAN) N-METHIONYL HUMAN GLIAL CELL LINE-DERIVED NEUROTROPHIC FACTOR (HUMAN)
- liatermide

Codes:
- CAS: 188630-14-0
- INN: 7885
- MERCK INDEX: M5880

Relationships: 1

Subunit: 2

Date approved: 2 years ago
Created: a few seconds ago
Last modified: a few seconds ago
Status: Validated (UNII)
Version: 1
Looking at the database (optional PgAdmin4)
localhost - ginas_db1 - public_ix_ginas_name

1. SELECT * FROM public_ix_ginas_name
2. ORDER BY uuid ASC LIMIT 100

<table>
<thead>
<tr>
<th>edited_by_id</th>
<th>deprecated</th>
<th>boolean</th>
<th>record_access</th>
<th>text</th>
<th>owner_uuid</th>
<th>Internal_references</th>
<th>name</th>
<th>full_name</th>
<th>std_name</th>
<th>type</th>
</tr>
</thead>
<tbody>
<tr>
<td>false</td>
<td>[binary data]</td>
<td>'false'</td>
<td>[binary data]</td>
<td>'false'</td>
<td>818be705-47c1-449c-a5c4-389444515f28</td>
<td>{'label': 'GinAS Reference'}</td>
<td>amcinonidum</td>
<td>[null]</td>
<td>amcinonidum</td>
<td>of</td>
</tr>
<tr>
<td>false</td>
<td>[binary data]</td>
<td>'false'</td>
<td>[binary data]</td>
<td>'false'</td>
<td>15c546df-5b29-407f-8e0c-9be43c1d69</td>
<td>{'label': 'GinAS Reference'}</td>
<td>dipivalyl epinephrine</td>
<td>[null]</td>
<td>dipivalyl epinephrine</td>
<td>en</td>
</tr>
<tr>
<td>false</td>
<td>[binary data]</td>
<td>'false'</td>
<td>[binary data]</td>
<td>'false'</td>
<td>7d440c45-03fe-4e80-a845-352d3f45c9</td>
<td>{'label': 'GinAS Reference'}</td>
<td>1-(5-hydroxy-5-methylhexyl) tiopero</td>
<td>[null]</td>
<td>1-(5-hydroxy-5-methylhexyl) tiopero</td>
<td>sys</td>
</tr>
<tr>
<td>false</td>
<td>[binary data]</td>
<td>'false'</td>
<td>[binary data]</td>
<td>'false'</td>
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<td>tiopero</td>
<td>[null]</td>
<td>tiopero</td>
<td>en</td>
</tr>
<tr>
<td>false</td>
<td>[binary data]</td>
<td>'false'</td>
<td>[binary data]</td>
<td>'false'</td>
<td>6f70f63b-80f8-4337-7a5b-3663af7e05</td>
<td>{'label': 'GinAS Reference'}</td>
<td>باركين</td>
<td>[null]</td>
<td>باركين</td>
<td>en</td>
</tr>
<tr>
<td>false</td>
<td>[binary data]</td>
<td>'false'</td>
<td>[binary data]</td>
<td>'false'</td>
<td>951c0a3a-44fa-4b87-9c6e</td>
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<td>باسولوزین</td>
<td>[null]</td>
<td>باسولوزین</td>
<td>en</td>
</tr>
<tr>
<td>false</td>
<td>[binary data]</td>
<td>'false'</td>
<td>[binary data]</td>
<td>'false'</td>
<td>1ec43b3a-2ee8-446e-952e</td>
<td>{'label': 'GinAS Reference'}</td>
<td>inosina</td>
<td>[null]</td>
<td>inosina</td>
<td>en</td>
</tr>
<tr>
<td>false</td>
<td>[binary data]</td>
<td>'false'</td>
<td>[binary data]</td>
<td>'false'</td>
<td>af5343a7-31bc-4950-bf4d-d06a96315f</td>
<td>{'label': 'GinAS Reference'}</td>
<td>茅萊洛</td>
<td>[null]</td>
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<td>en</td>
</tr>
<tr>
<td>false</td>
<td>[binary data]</td>
<td>'false'</td>
<td>[binary data]</td>
<td>'false'</td>
<td>5b9d2dce-8875-4e8a-9b9b-7a4b516a73</td>
<td>{'label': 'GinAS Reference'}</td>
<td>isoosuprina</td>
<td>[null]</td>
<td>isoosuprina</td>
<td>en</td>
</tr>
<tr>
<td>false</td>
<td>[binary data]</td>
<td>'false'</td>
<td>[binary data]</td>
<td>'false'</td>
<td>701f7e6e-76a2-48a5-8373</td>
<td>{'label': 'GinAS Reference'}</td>
<td>MALARONE COMPONENT</td>
<td>[null]</td>
<td>MALARONE COMPONENT</td>
<td>en</td>
</tr>
</tbody>
</table>
Kill the ginas process

In another terminal window ...

```
welscha@kale:~/Documents/gin2s2/gsr2.0h2$ ./bin/ginas -Dconfig.file=conf/gin2s2.conf -J-Xmx4G
Play server process ID is 15766
Initializing
welscha@kale:~/Documents/gin2s2/gsr2.0h2$
```

```
welscha@kale:~$
welscha@kale:~$
welscha@kale:~$ kill -SIGTERM 15766
welscha@kale:~$
```
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========================================================================
*** STEP 1. Get background information and instructions on the NCATS site
========================================================================
https://tripod.nih.gov/ginas/#/gsrs/release
(There are instructions if you scroll down!)

Requirements:
4-core (+) CPU
8GB (+) Memory
100GB (+) hard drive
Java 8

For our purposes, the evolutions step should be skipped.

================================================================
*** STEP 2. Download the public Ginas version and example data.
================================================================
See: https://tripod.nih.gov/ginas/#/gsrs/release
Open a Linux terminal window and issue the following commands:

myuser%> cd
myuser%> mkdir ginas2
myuser%> cd ginas2
myuser%> wget https://tripod.nih.gov/ginas/releases/gsrs2_0_beta_bundled_h2_smallseed.zip
myuser%> unzip gsrs2_0_beta_bundled_h2_smallseed.zip
myuser%> wget https://tripod.nih.gov/ginas/releases/smallSeedData.gsrs
myuser%> cd gsr2.0h2
myuser%> ls  # to see contents

=================================================================
*** STEP 3. INSTALL POSTGRESQL
=================================================================
(From: https://tecadmin.net/install-postgresql-server-on-ubuntu/)
myuser%> cd
myuser%> mkdir temp-pg
myuser%> cd temp-pg
myuser%> wget -q https://www.postgresql.org/media/keys/ACCC4CF8.asc -O - | sudo apt-key add -
myuser%> sudo sh -c 'echo "deb http://apt.postgresql.org/pub/repos/apt/ `lsb_release -cs`-pgdg main" >> /etc/apt/sources.list.d/pgdg.list'
myuser%> sudo apt-get update
myuser%> sudo apt-get upgrade
myuser%> sudo apt-get install postgresql postgresql-contrib
myuser%> cd

## If all goes well, a linux operating system "postgres" user now exists.

myuser%> sudo su - postgres
==> gets you to that account temporarily.
postgres%> exit
==> to get back to your own user account.

myuser%

## Go back into the postgres account and start "psql" --- the command line interface.

myuser%> sudo su - postgres
postgres%> psql
postgres=# \password postgres  ## I set it to hello4
postgres=# \q

=======================================================
*** STEP 4. Create the Ginas database and database user
=======================================================

postgres%> psql
## You're now in the postgres CLI.
## Issue the following commands to create a Ginas user and database.
## You can use whatever user/database/password you want.
postgres-# create user ginas_usr with password 'hello5';
postgres-# create database ginas_db;
postgres-# grant all privileges on database ginas_db to ginas_usr;
postgres-# \q
postgres%> exit
myuser%

==================================================================
*** STEP 5. MAKE Postresql open to local accounts on the computer.
==================================================================
## Change your PostresSQL configuration to allow local access to the Postgresql database.
myuser%> sudo nano /etc/postgresql/10/main/pg_hba.conf

    ## Change the Posgres Configuration to allow local connections
    ## Chnage FROM:
    local  all    all    peer
    ## TO:
    local  all    all    md5
    ## Control-X to quit nano.
    ## then restart Postgresql Server
myuser%> sudo service postgresql restart

## Now, check if we can access database with psql. Notice we are doing it directly from myuser%
myuser%> psql -U ginas_usr -d ginas_db -W
ginas_db=>>
## try \l to list databases, the quit.

ginas_db=> \l
ginas_db=> \q

===================================================================
*** STEP 6. Change your ginas configuration to specify PostgreSQL.
===================================================================

myuser%> cd
myuser%> cd ginas2/gsr2.0h2
myuser%> nano ./conf/ginas.conf

Add the following at the END.

```
#postGreSQL example
db.default.driver="org.postgresql.Driver"
db.default.url="jdbc:postgresql://localhost:5432/ginas_db"
db.default.user="ginas_usr"
db.default.password="hello5"
END postGreSQL example
```

=====
*** STEP 7. Run Ginas
=====

myuser%> ./bin/ginas -Dconfig.file=conf/ginas.conf -J-Xmx4G
## ... or
myuser%> nohup ./bin/ginas -Dconfig.file=conf/ginas.conf -J-Xmx4G

## Take note of the process ID after so you can stop it later.
## When the program is done initializing ==> in your browser load:
http://localhost:9000/ginas/app

## Click on the Admin link, login with credentials.

```
   user: admin
      password: admin
```

## If this is your first time, you'll have no data and you'll have to import it.

a) click on admin in the TOP menu (next to "sequence search")
b) click on data management
c) In the file dialog, navigate to the file smallSeedData.gsrs you downloaded earlier and click on the load button. Loading will take a while. You don't have to load everything if you just want to see if it worked. After loading some substances, you'll be able to browse substances by clicking on the Substances Link.

============
*** STEP 7. Quit Ginas
============

## When you want to end the process gracefully:

myuser%> kill -SIGTERM YOUR_PROCESS_ID

=============
*** ERRORS YOU MIGHT GET
============
In some attempts, the Play framework seemed to hang or complained about file locks. I made things work by clearing the cache directory (.ginas.ix/cache). However, there maybe consequences contend with if you do that.

Database 'default' is in an inconsistent state with postgresql driver.
==> I got this when I first tried to install and maybe things didn't complete with the database population. The remedy was to drop the database and recreate it as in Step 4

Oops, cannot start the server.
org.jboss.netty.channel.ChannelException: Failed to bind to: /0.0.0.0:9000
==> find the PID for the process running play framework with ==> ps auxwww | grep play ==> then ==> kill -9 YOUR_PIDI

After running ginas, screen hangs and says "Initializing" forever.
(It may not tell you it's done initializing, so if you've been staring at a blank screen that says "initializing" for a while, try loading http://localhost:9000/ginapp in your server. )

==========
*** Links
==========

https://tripod.nih.gov/ginapp/#/gsrs/
https://help.ubuntu.com/community/AptGet/Howto
https://medium.com/coderscorner/installing-oracle-java-8-in-ubuntu-16-10-845507b13343
https://tecadmin.net/install-postgresql-server-on-ubuntu/
http://suite.opengeo.org/docs/latest/dataadmin/pgGettingStarted/firstconnect.html
https://www.ntchosting.com/encyclopedia/databases/postgresql/create-user/
https://askubuntu.com/questions/831262/how-to-install-pgadmin-4-in-desktop-mode-on-ubuntu
(see Victor's answer)

Once you've installed it, start it again, like so:
  ## cd ~/pgadmin4
  ## source bin/activate
  ## python lib/python2.7/site-packages/pgadmin4/pgAdmin4.py


==========
*** Explore API
==========

https://tripod.nih.gov/ginapp/#/gsrs/api#details
https://tripod.nih.gov/ginapp/app/api/v1