Dockerized Galaxy for Tool Publishing

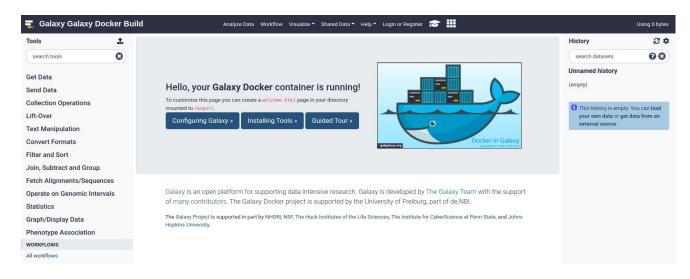
Galaxy Resources for Tools Developers Webinar May 12th, 2021 Anthony Bretaudeau - GenOuest - Rennes, France

Galaxy Docker image

Docker image to launch Galaxy in seconds:

docker run -d -p 8080:80 quay.io/bgruening/galaxy:20.09

...then browse to http://localhost:8080/



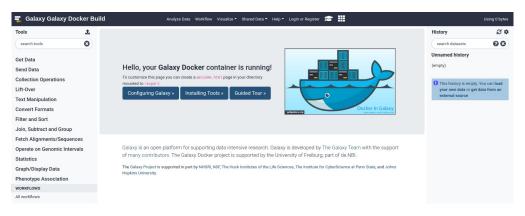
Galaxy Docker image

Image based on Ubuntu 18.04 LTS

Embeds the Galaxy web app + PostgreSQL db + ftp server + Reports web app...

Persist all data by mounting a single directory: /export/

https://github.com/bgruening/docker-galaxy-stable

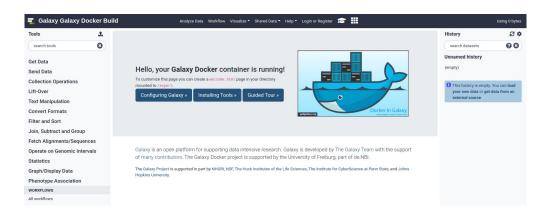


Galaxy Docker image

Configure by setting environment variables

Jobs run inside the container by default, but can be configured to run externally

Comes with default Galaxy Tools



Galaxy Flavours

Docker images with preinstalled tools, workflows, data

Examples:

- RNA Workbench
- Genome Annotation
- Metagenomics
- Proteomics
- Imaging
- Workflow4Metabolomics
- HiCExplorer
- deepTools
- ...

List on https://github.com/bqruening/docker-galaxy-stable#list-of-galaxy-flavours--toc

How to create your own?

Tools install

Tool list in standard YAML format

"install-tools" command inside the container

install-tools /path/to/tool_list.yml

```
api_key: admin
galaxy_instance: http://localhost:8080
install resolver dependencies: true
install tool dependencies: false
tools:
# RNA Alignment
- name: compalignp
  owner: rnateam
  tool_panel_section_label: "RNA Alignment"
- name: mafft
  owner: rnateam
  tool panel section label: "RNA Alignment"
- name: suite_locarna
  owner: rnateam
  tool_panel_section_label: "RNA Alignment"
- name: locarna_multiple
  owner: rnateam
  tool_panel_section_label: "RNA Alignment"
  revisions:
    - 8414fea2a6fd
```

Workflows install

Workflows in .ga format, downloaded from a Galaxy instance

"workflow-install" command inside the container

```
workflow-install --workflow_path /path/to/workflows/ -g \
http://localhost:8080 -u $GALAXY_DEFAULT_ADMIN_USER -p \
$GALAXY_DEFAULT_ADMIN_PASSWORD
```

Populating data libraries

Data library content in standard YAML format

"setup-data-libraries" command inside the container

```
setup-data-libraries -i /path/to/library_data.yaml -g \
http://localhost:8080 -u $GALAXY_DEFAULT_ADMIN_USER -p \
$GALAXY_DEFAULT_ADMIN_PASSWORD
```

Running Data Managers

Data manager runs in standard YAML format

```
data_managers:
    # Data manager ID
    - id: toolshed.g2.bx.psu.edu/repos/devteam/data_manager_fetch_genome_dbkeys_all_fasta/data_manager_fetch_genome_all_fas
      # tool parameters, nested parameters should be specified using a pipe (|)
      params:
          - 'dbkey source|dbkey': '{{ item }}'
          - 'reference_source|reference_source_selector': 'ucsc'
          - 'reference source|requested dbkey': '{{ item }}'
      # Items refere to a list of variables you want to run this data manager. You can use them inside the param field with
      # In case of genome for example you can run this DM with multiple genomes, or you could give multiple URLs.
      items:
          - mm10
          - dm3
      # Name of the data-tables you want to reload after your DM are finished. This can be important for subsequent data ma
      data table reload:
          - all fasta

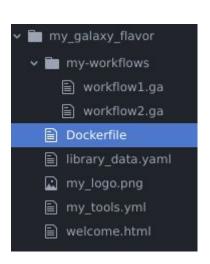
    dbkeys
```

"run-data-managers" command inside the container

```
run-data-managers --config /path/to/data_manager_rna_seq.yaml -g \
http://localhost:8080 -u $GALAXY_DEFAULT_ADMIN_USER -p \
$GALAXY_DEFAULT_ADMIN_PASSWORD
```

Creating your own Galaxy Flavours

Create your own Docker image, based on quay.io/bgruening/galaxy



```
FROM quay.io/bgruening/galaxy:20.09
ENV GALAXY CONFIG BRAND="My own flavor"
ADD my tools.yml $GALAXY ROOT/tools.yaml
RUN install-tools $GALAXY ROOT/tools.yaml
ADD library data.yaml $GALAXY ROOT/library data.yaml
RUN setup-data-libraries -i $GALAXY ROOT/library data.yaml -g http://localhost:8080 \
    -u $GALAXY DEFAULT ADMIN USER -p $GALAXY DEFAULT ADMIN PASSWORD
ADD ./my-workflows/* $GALAXY HOME/workflows/
RUN workflow-install --workflow path $GALAXY HOME/workflows/ -q http://localhost:8080 \
    -u $GALAXY DEFAULT ADMIN USER -p $GALAXY DEFAULT ADMIN PASSWORD
ADD my logo.png $GALAXY CONFIG DIR/web/welcome image.png
ADD welcome.html $GALAXY CONFIG DIR/web/welcome.html
```

Creating your own Galaxy Flavours

Create your own Docker image, based on quay.io/bgruening/galaxy

Build locally (docker build)

or make it public on GitHub and have it built by hub.docker.com or quay.io

Galaxy Training Network Docker images

All tutorials in GTN have a corresponding Docker image built automatically

Galaxy instances

You can use a public Galaxy instance which has been tested for the availability of the used tools. They are listed along with the tutorials above.

You can also use the following Docker image for these tutorials:

docker run -p 8080:80 quay.io/galaxy/assembly-training

NOTE: Use the -d flag at the end of the command if you want to automatically download all the data-libraries into the container.

It will launch a flavored Galaxy instance available on http://localhost:8080. This instance will contain all the tools and workflows to follow the tutorials in this topic. Login as admin with password password to access everything.