Galaxy Pasteur

Patchwork of experiences and improvements

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Summary

Part 0 : Galaxy Pasteur

Part 1 : Adaptations to the Pasteur infrastructure

- Module
- “Libraries” automation
- Galaxy reporting

Part 2 : Problems and corrections

- I/O Problems
- Purged User Problem

Part 3 : Future improvements

- Upload submitted for remote execution
- Statistics on Galaxy reporting
- SynBioWatch Project

Galaxy Pasteur

At Institut Pasteur, Galaxy consists in:

- An instance used by 133 users and administrated by 1.5 fte administrators.
- A ToolShed with 89 repositories containing 289 tools.
- An average of 1783 jobs per month since February 2013.
- Trainings on Galaxy, twice a year.
- Trainings using Galaxy, twice a year.

Adaptations to the Pasteur infrastructure

“Libraries” automation

- Why automate library creation?
  - Private data to deal with,
  - Only 1.5 fte administrators,
  - Big data upload and export.

- New API script `scripts/api/automate_library.py` , how it works:
  - Root cron script execution with admin API key (launched every 10 minutes)
  - Retrieves the users list using the API
  - Checks if the exchange directories exist for each user
  - If not, creates a Galaxy library named `“login”` using the API and creates 2 directories `export/”login” upload/”login”` with the right linux permissions
  - Sends an email to admins who modify the library permission (by hand)

- Clarifications:
  - Deals also with linux permissions of exported files.
  - User `cp/scp` the data in `upload/”login”` and upload in Galaxy through the interface.

Adaptations to the Pasteur infrastructure

Module

- Module provides a way to dynamically modify of a user’s environment.
  - Uses modulefiles
  - Allows the management of several packages/software versions on the same instance

- Patches on `/lib/galaxy/` directory:
  - `config.py ;`
  - `jobs/__init__.py ;`
  - `jobs/runners/__init__.py ;`

- How it works:
  - A `module_conf.xml` file lists tool ids and their associated modules:

```
<tool id="tophat2" version="2.0.7" module="tophat/2.0.7" />
```

  - When the tool is launched, Galaxy uses the tool `id` to retrieve the list of modules
  - Then, Galaxy creates a `module.sh` script to load the modules

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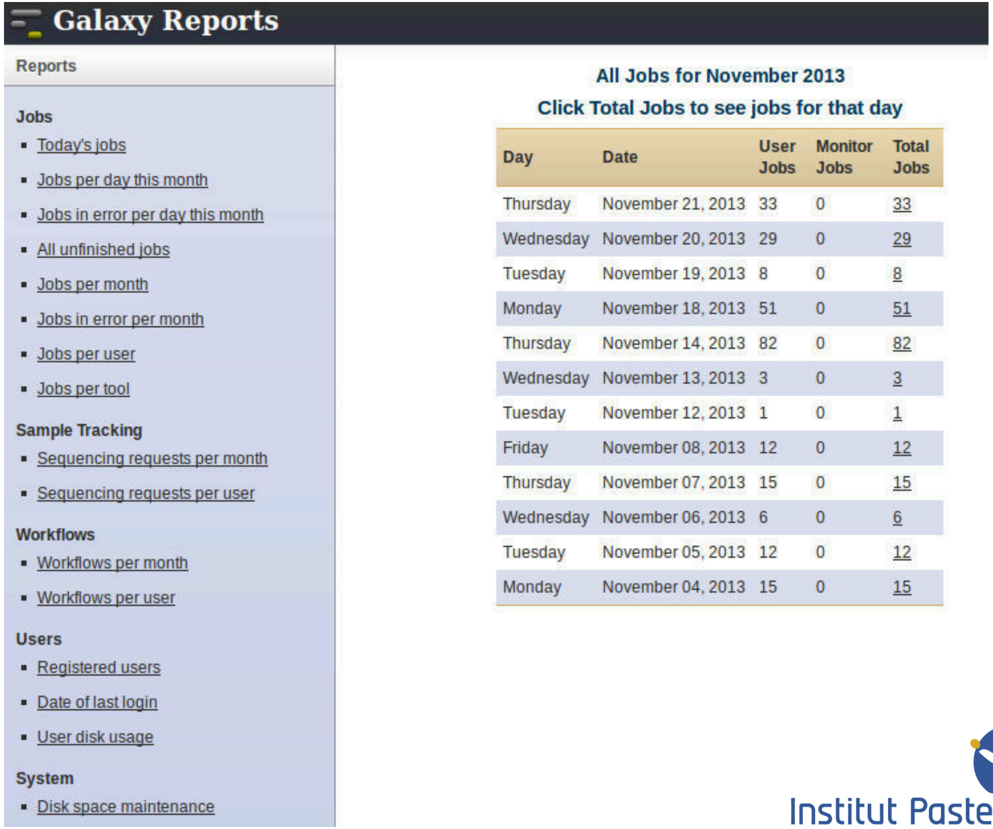
Adaptations to the Pasteur infrastructure

Galaxy reporting

- Natively in Galaxy
- Setup equivalent to ToolShed
- Provides many interesting metrics
    - Jobs per month
    - Jobs per user
    - Jobs per tool
    - User disk usage
    - ...



Galaxy Reports

Reports

Jobs

- Today's jobs
- Jobs per day this month
- Jobs in error per day this month
- All unfinished jobs
- Jobs per month
- Jobs in error per month
- Jobs per user
- Jobs per tool

Sample Tracking

- Sequencing requests per month
- Sequencing requests per user

Workflows

- Workflows per month
- Workflows per user

Users

- Registered users
- Date of last login
- User disk usage

System

- Disk space maintenance

All Jobs for November 2013

Click Total Jobs to see jobs for that day

Day	Date	User Jobs	Monitor Jobs	Total Jobs
Thursday	November 21, 2013	33	0	33
Wednesday	November 20, 2013	29	0	29
Tuesday	November 19, 2013	8	0	8
Monday	November 18, 2013	51	0	51
Thursday	November 14, 2013	82	0	82
Wednesday	November 13, 2013	3	0	3
Tuesday	November 12, 2013	1	0	1
Friday	November 08, 2013	12	0	12
Thursday	November 07, 2013	15	0	15
Wednesday	November 06, 2013	6	0	6
Tuesday	November 05, 2013	12	0	12
Monday	November 04, 2013	15	0	15

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Problems and corrections

I/O Problems

- Identification of two I/O intensive process
  - Galaxy renaming step for output files (output --> dataset)
  - Execution of `set_metadata.sh` script which collects metadata information

- Patches on:
  - `lib/galaxy/jobs/runners/__init__.py`
  - `set_metadata.sh`

- How it works:
  - `cp` and `rm` commands are replaced by `mv` command (faster on the same file system)
  - `set_metadata.py` script executed on cluster nodes

Problems and corrections

Purged User problem

- There and back again at Pasteur (No way to unpurge a user)
  - A user left the Institut Pasteur (purged) and got back a month later.
  - Impossible to unpurge the user

- Modified API script:
  - `scripts/cleanup_datasets/pgcleanup.py`

- How it works:
  - New function, operating directly on the Galaxy database
  - Purged and Deleted attributes for that user are changed from `true` to `false`

```
update galaxy_user set purged='f', deleted='f' where id in (select id from
galaxy_user where email='%s');
```

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Future improvements

Remote execution of big data uploads

- Galaxy mainly used for NGS analysis.

- Another I/O intensive process is the upload of big files
  - For the moment, the process is run on the web server (head)
  - Upload is handled like a Galaxy tool, xml + script

- Idea: patch `tools/data_source/upload.py, tools/data_source/upload.xml`
  - We need to differentiate the upload possibilites (`http` and `cp` from `upload/”login”`)
  - Identify file system uploads and remotely execute them on the cluster
  - We are testing this solution

Future improvements

Other points

- Galaxy reporting
  - More statistics are needed
    - automation of data retrieval from Galaxy reporting
    - graphics generation
  - Project:
    - scripts development to automate it
    - use of Galaxy API to retrieve data
- Tool ID with ToolShed
  - too long name (full path of ToolShed directory)

`galaxy.web.pasteur.fr/toolshed-pasteur/repos/fmareuil/gatk2/gatk2_base_recalibrator/0.0.4`

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Future improvements

Collaborative project at Institut Pasteur

- The PGP (Pôle de Génotypage des Pathogènes) group is implementing a specific web interface to facilitate the management of their analysis to detect pathogens within NGS sequences samples:
  - It contains a LIMS database and a result exploratory interface
  - It is launched on a web server linked to Institut Pasteur infrastructure.
  - It communicates remotely with Galaxy to execute pre-built analysis workflows.

- Our contribution is to help building the remote communication with Galaxy API. They need to:
  - Copy (big) data within Galaxy environment, (ok)
  - Upload those data into Galaxy libraries (ok)
  - Import those libraries content into Galaxy histories (almost ok)
  - Launch the workflows (fixed or tunable options) (not yet)
  - Export the results (not yet)

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Acknowledgments

Galaxy Day team

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Yes for an unified Galaxy WIKI!!

PGP group

E&I team