Galaxy on a cluster: user & project management

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Prerequisites

- VirtualBox?

- UsersProjects Galaxy VM downloaded?
  - http://folk.uio.no/nikolaiv/GCC2014-Users-Projects.ova

Password: UsersProjects2014
What are the main cluster features, and requirements?

- Running jobs on a cluster is expensive, requires plenty of resources (processors, disk space, bandwidth, electricity (yes, the bills are impressive), and ... daily human expertise)
- Clusters are like banks, they are structured with regard to:
  - **users**: average unix-type users
  - **accounts** (projects): users belong to accounts
  - **allocations** (granted to each account) which control:
    - time span validity, e.g. 30:12:2014 - 02:02.2015
    - use of CPU resources, e.g. 1 000 000 CPU hours
    - use of machines: number and type
    - job priorities
    - etc.
Clustering and/or Galaxy?

or what are our challenges with regard to user DBs

**Cluster**

- require complex user DB management
- user DBs are usually dependent on other services responsible for user accounts (LDAP)

**Galaxy**

- has a “user-managed” user DB
- does not control user's affiliation at registration

A very common situation:

- Cluster users: in `/home`
- Galaxy users: Only in Galaxy DB
- Cluster & Galaxy users: both in Galaxy DB and in `/home`

problematic
Clusters and/\textit{vs} Galaxy?

or what are our challenges with regard to resource allocation

\begin{itemize}
  \item Cluster
    \begin{itemize}
      \item has an integrated accounting system that tracks and manages resource usage
      \item all cluster users are organized into accounts with respective allocations
    \end{itemize}
  \item Galaxy
    \begin{itemize}
      \item does not have any accounting system
      \item the only resource limitations are disk quotas
    \end{itemize}
\end{itemize}
Clusters not vs but with Galaxy
a possible (and working) solution

- all galaxy jobs sent to the cluster belong to one single user: *galaxy*

- information about each Galaxy job is propagated to the cluster and back to Galaxy when finished; it contains
  - Information about the required/used resources: number of cpu, job duration, memory, etc.
  - Galaxy and Cluster job id
  - Information about the real job owner

- the job data is handled by a separate allocation manager (GOLD) which charges the account of the real Galaxy user
Clusters and Galaxy: the strategy in (technical) detail

1. (simultaneously) user registered in Galaxy user DB

2. job

3. check for available resources in GOLD

4. confirmation for available resources from GOLD, resources reserved

5. job sent to cluster, all job parameters included

6. completed job info sent to Galaxy, results displayed in history panel

7. job data sent to GOLD, account charged

* all job parameters sent to the cluster

Job running -> Job completed

GOLD allocation manager

a. user registered in GOLD user DB

b. user associated to an account in GOLD

c. user receives an allocation within the account

galaxy

user

registered in Galaxy user DB

user launches a job to be executed on the cluster

cluster

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Clustering + Galaxy:
what is this tutorial about

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Clusters + Galaxy: what is this tutorial about

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GOLD installation and configuration

Galaxy customization: communication with GOLD

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b. user associated to an account in GOLD

c. user receives an allocation within the account

user registered in Galaxy user DB

GOLD allocation manager

Job running -> Job completed

all job parameters sent to the cluster

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Clusters + Galaxy: what is this tutorial about

**GOLD installation and configuration**

1. User registered in Galaxy DB
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**Galaxy customization: communication with GOLD**

**Galaxy customization: communication with the cluster**

**GOLD allocation manager**

- A. User registered in GOLD user DB
- B. User associated to an account in GOLD
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**Job running -> Job completed**

**drmaa libraries**

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GOLD Allocation Manager
http://docs.adaptivecomputing.com/gold/

- open source L(A)PP technology
  - Linux
  - Apache (optional, needed for GUI only)
  - Postgresql (MySQL)
  - Perl
- easy to install (compilation needed)
- terminal and GUI (optional)
  - easy to plug into Galaxy – gold commands are called as subprocesses in python
- excellent manual
- v2.2.0.5 at present, project stopped, the resumed, now 3.x available

Setup instructions in the file GOLD-core-installation.txt


```bash
[root@galaxy-prod01 ~]# /opt/gold/bin/glsuser | grep added
abegiz3@yahoo.com     True                      non-feide user added by magnus.popp@hnm.uio.no
anna.vader@unis.no    True   Anna Vader  anna.vader@unis.no  Manually added non-feide project manager - nikolaiv
laurindodasilva@fas.harvard.edu True
mgrabowsk@email.gwu.edu True                      non-feide user added by t.f.hansen@ibv.uio.no
ovidiu.paun@univie.ac.at True                      non-feide user added by a.k.brysting@ibv.uio.no
ricivito@hotmail.it   True                      non-feide user added by geirksa@ifi.uio.no
```
GOLD integration into Galaxy: a new feature

**Users:**

- Apply for a project (account) specifying the necessary resources:
  - project duration
  - total of cpu hours
  - preferred applications on the cluster
- After their project approval, the users become Project Managers for their project

**Project managers:**

- Manage the projects:
  - delete
  - prolong
  - modify: cpu hours, apps
  - see pending/rejected projects
- Add users to the projects
Project application form

Lifeportal project application form

Please fill in the required information

Personal information about the project leader

Project responsible, e.g. John Doe, (permitted chars: capital/small letters and blanks)*.
Job title/position (permitted chars: capital/small letters, digits and blanks):
E-mail address: na.vazov@hus.uio.no
Phone no. (please, use digits only, e.g. 0047XX for Norway):
Cell phone number (please, use digits only, e.g. 0047XX for Norway)*.
Institution (Faculty, Department) (permitted chars: capital/small letters and blanks)*.
Country (permitted chars: capital/small letters and blanks)*.

Project information

Project name (permitted chars: capital/small letters and digits)*.
CPU hours (specify how many CPU hours you need for the project) (permitted chars: digits)*.
Preferred applications* (Click on the box to display the apps):
BEAST
Blast
Gaussian
Migrate

Project description (permitted chars: all)*:

Start date:
End date:
YYYY-MM-DD
2014-09-30

I declare that the project does not contain sensitive data*
I have read the Lifeportal requirements and accepted them*

*Note: Fields marked * must be filled out.

Send application form  Cancel
Project selection for job execution
Project management

<table>
<thead>
<tr>
<th>Project owner</th>
<th>Project name</th>
<th>Users</th>
<th>Active</th>
<th>Amount</th>
<th>Description</th>
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<td>2014-09-30</td>
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</tbody>
</table>
GOLD integration into Galaxy: code modification

Python scripts

Makos

Setup instructions in the file Galaxy-GOLD-code.txt
Sending Galaxy jobs to the cluster: chart

- **drmaa.py** (Galaxy)
- **Drmaa-python.egg** (Galaxy)
- **DRMAA C-library**
- **SLURM**

**Job authorisation from GOLD**

**Account charged in GOLD**

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Sending Galaxy jobs to the cluster
see configuration files on the VM

- **SLURM client / munge** must be installed and started (running)

- **DRMAA C-library** must be edited and recompiled to accept the modified switches

- **drmaa.py** and **drmaa-python.egg** must be edited to account for all necessary SLURM switches
SLURM / MUNGED client installation
(SLURM manager is already installed on the cluster)

- `apt-get install munge`
- `apt-get install slurm-llnl`
- `apt-get install libslurm-dev`
- `/usr/sbin/create-munge-key`
- `/etc/init.d/munge start`

Setup instructions in the file
MUNGEG-SLURM-DRMAA-installation.txt
DRMAA C-library

DRMAA C-library is a mediator between drmaa.py/drmaa.egg and SLURM queueing system

- Copy from /site/drmaa/slurm-drmaa-1.0.6 on the supplied VM or
- download from http://apps.man.poznan.pl/trac/slurm-drmaa

Setup instructions given in the file MUNGE-SLURM-DRMAA-installation.txt
Galaxy code modification for DRMAA-SLURM

Python scripts

[root@galaxy-prod01 BaltimoreVM]# tar tvf drmaa_pythons.tar
-rw-r-xr-- root/root     20108 2014-06-11 14:20 drmaa.py
-rw-r-xr-- root/root     26474 2014-06-11 14:19 galaxy_tools_actions_init_.py
-rwxr-xr-x root/root    182793 2014-06-11 14:17 galaxy_tools_init_.py
-rw-r-xr-- root/root      7477 2014-06-11 14:20 mapper.py

Makos

[root@galaxy-prod01 BaltimoreVM]# tar tvf drmaa_makos.tar

Setup instructions in the file
Galaxy-DRMAA-code.txt

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What do we send and what do we receive?

To the cluster

```bash
>>> DRMAA.PY slurm script #!/bin/sh
#SBATCH -A nn9108k
#SBATCH -t 300:00:00
#SBATCH -D /work/projects/galaxy/data/database_galaxy_prod01/job_working_directory/000/629
#SBATCH -J a.k.krabberod@ibv.uio.no::lp2
#SBATCH -n 1
#SBATCH --mem-per-cpu=4000
#SBATCH --ntasks-per-node=8
#SBATCH --partition=normal

source /etc/profile
source /cluster/bin/jobsetup

cd /work/projects/galaxy/data/database_galaxy_prod01/job_working_directory/000/629
module load blast+
blastn -query "/work/projects/galaxy/data/database_galaxy_prod01/files/000/dataset_922.dat" -db "/work/databases/bio/ncbi-pre/est_others" -task blastn -evalue 0.001 -out
/work/projects/galaxy/data/database_galaxy_prod01/files/000/dataset_924.dat -outfmt 6 -num_threads 8 -dust yes -strand both -max_target_seqs 100

echo $? > /work/projects/galaxy/data/database_galaxy_prod01/job_working_directory/000/629/galaxy_629.ec
```

From the cluster

```json

{"charge_duration": '451587',
'galaxy_job_id': '629',
'lifeportal_project': 'lp2',
'machine': 'c17-6',
'processes': '8',
'slurm_account': 'nn9108k',
'slurm_job_id': '5200757',
'user': 'a.k.krabberod@ibv.uio.no'}

Successfully charged job 629 for 3612696 credits – MESSAGE FROM GOLD

galaxy.jobs.runners.drmaa DEBUG 2014-02-27 20:27:26,034 Successfully charged job 629 for 3612696 credits
galaxy.jobs.runners.drmaa DEBUG 2014-02-27 20:27:26,034 (629/5200757) state change: job finished normally
```
Application integration

- Applications can be executed locally or on the cluster
- Cluster apps installed on the cluster file system under *module* software environment management
- "module load" statement included in the *xml command block*
- Galaxy internal tools/libraries were exported on the cluster (all /galaxy-dist/lib tree) and dependencies installed
Work plan

- Go through the files in the VM
  - README-FIRST.txt (in the Desktop>Setup_Manual)
  - Login / version info file
  - general setup files
  - GOLD setup files
  - Galaxy-GOLD related changes
  - Galaxy-DRMAA related changes

- Run the feature on the VM (Galaxy interface)
  - Start all the services
    - sudo -u daemon munged
    - slurmctld
    - slurmd
    - /opt/gold/sbin/goldd start
    - cd /home/galaxy/galaxy-dist
    - ./run.sh --daemon
    - type "localhost" for the URL (in a browser)

- DEBUG
  - tail -f /home/galaxy/galaxy-dist/paster.log

- register, log in, apply for a project, approve a project, GOLD and Galaxy Web

- An example from a production setup (Lifeportal)
Overview

Abel cluster
10000+ cores :: 258 Teraflops/s :: 40 TebiBytes :: FhGFS

FhGFS partitions mounted on the VM

services

External authentication (FEIDE)
Locally registered users

Apache proxy

External authentication (FEIDE)
Locally registered users

Apache proxy

Interface between Galaxy and SLURM – DRMAA job scheduler - SLURM

Interface between Galaxy and SLURM – DRMAA job scheduler - SLURM

SSL connection

Galaxy Web server (WSGI)

Filesender (big file upload)

GOLD allocation manager

PostgreSQL DB server:
1. Galaxy User DB
2. GOLD DB
3. Filesender DB

DATABASE HOTEL

1. Galaxy User DB
2. GOLD DB
3. Filesender DB
Detailed setup page for our production server can be found here:


Write to us at:

lifeportal-help@usit.uio.no

Link to our production server:

http://lifeportal.uio.no