

# The Galaxy Toolshed

[usegalaxy.org/toolshed](http://usegalaxy.org/toolshed)





# The Galaxy API

# API Foundation

- Technologies
  - Representational State Transfer (REST)
    - Sessionless operations via HTTP
  - JavaScript Object Notation (JSON)

GO

# Other API Interfaces

- Library permissions
- Forms
- Sample tracking requests and samples
- Manage users, roles, and quotas
- Execute tools and workflows

# End-to-end pipelines

- Automatically upload data retrieved from instruments
- Start a workflow
- Move outputs to a data library



# Beneath the Clouds

Building your own Galaxy production service

[usegalaxy.org/production](https://usegalaxy.org/production)

# Galaxy runs out of the box!

- Simple download, setup, and install design:

```
% hg clone ...
```

```
% sh run.sh
```

- Great for development!
- Not designed to support multiple users in a production environment with default configuration



# Development-oriented defaults

- SQLite database
- One process
- Built-in HTTP server
- Local job execution

# Start Fresh

- Don't use an old Galaxy installation - check out a new copy
- Use a dedicated **non-root** user
- Start and stop with your OS' system service method (e.g. init.d, service)
- Don't share the database or database user
- Use a dedicated Python or **virtualenv**
- If you plan to use a cluster, put galaxy in a shared filesystem

# Galaxy Config Basics

- Use the sample config (copy before starting):
  - `% cp universe_wsgi.ini.sample universe_wsgi.ini`
  - Read the full sample config
- Set:
  - `use_interactive = False` - Not even safe (exposes config)
  - `debug = False` - You'll still be able to see tracebacks in the log file, doesn't load response in memory

```
# ---- Galaxy -----  
  
# Configuration of the Galaxy application.  
  
[app:main]  
  
# By default, Galaxy uses a SQLite database at 'database/universe.sqlite'. You  
# may use a SQLAlchemy connection string to specify an external database  
# instead. This string takes many options which are explained in detail in the  
# config file documentation.  
#database_connection = sqlite:///./database/universe.sqlite  
database_connection = postgres:///galaxy  
  
# -- Data Libraries  
  
# These library upload options are described in much more detail in the wiki:  
# http://wiki.g2.bx.psu.edu/Admin/Data%20Libraries/Uploading%20Library%20Files  
  
# Add an option to the library upload form which allows administrators to  
# upload a directory of files.  
#library_import_dir = None  
library_import_dir = /Users/nate/import
```

# Galaxy Admin Interface

Galaxy Administration  
https://main.g2.bx.psu.edu/admin

Galaxy

Analyze Data

Workflow

Shared Data

Lab

Visualization

Admin

Help

User

Using 62.4 Gb

## Administration

### Security

- [Manage users](#)
- [Manage groups](#)
- [Manage roles](#)

### Data

- [Manage quotas](#)
- [Manage data libraries](#)

### Server

- [Tool versions](#)
- [Reload a tool's configuration](#)
- [Profile memory usage](#)
- [Manage jobs](#)
- [Manage installed tool shed repositories](#)

### Tool sheds

- [Search and browse tool sheds](#)

### Form Definitions

- [Manage form definitions](#)

### Sample Tracking

- [Manage sequencers and external services](#)
- [Manage request types](#)

## Administration

The menu on the left provides the following features

- **Security** – see the **Data Security and Data Libraries** section below for details
  - **Manage users** – provides a view of the registered users and all groups and non-private roles associated with each user.
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- **add library item** – Users that have the role can add library items to this data library or folder

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The left navigation menu is expanded to show the "Server" section, which includes the following items:

- [Tool versions](#)
- [Reload a tool's configuration](#)
- [Profile memory usage](#)
- [Manage jobs](#)
- [Manage installed tool shed repositories](#)

The main content area is titled "Administration" and contains the following text:

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- **Data**
  - **Manage data libraries** – allows administrators to create, edit, and delete data libraries. Administrators can also upload datasets into a data library. Currently, only administrators can create data libraries. When a data library is first created, it is considered "public" since it will be displayed in the "Data Libraries" view for any user, even those that are not logged in. The Galaxy administrator can restrict access to a data library by associating roles with the data library's "access library" permission. This permission will conservatively override the [dataset] "access" permission for the data library's contained datasets. For example, if a data library's "access library" permission is associated with Role1 and the data library contains "public" datasets, the data library will still only be displayed to those users that have Role1. However, if the data library's "access library" permission is associated with both Role1 and Role2 and the data library contains datasets whose [dataset] "access" permission is associated with only Role1, then users that have Role2 will be able to access the library, but will not see those contained datasets whose [dataset] "access" permission is associated with only Role1. In addition to the "access library" permission, permission to perform the following functions on the data library (and it's contents) can be granted to users (a library item is one of: a data library, a library folder, a library dataset).
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# Galaxy Admin Interface

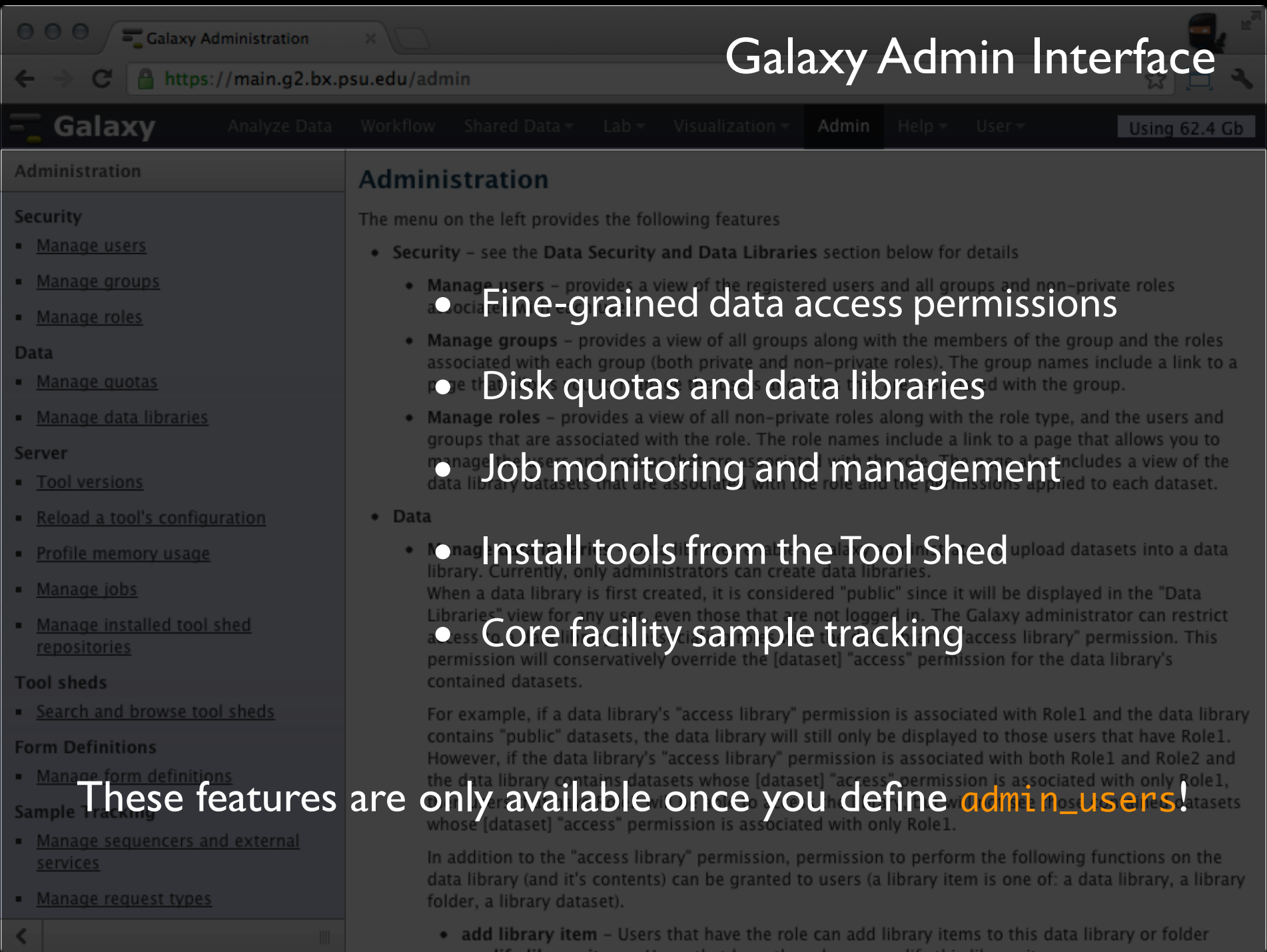
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**Administration**

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- **Security** – see the **Data Security and Data Libraries** section below for details
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    - **Fine-grained data access permissions**
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    - **Disk quotas and data libraries**
  - **Manage roles** – provides a view of all non-private roles along with the role type, and the users and groups that are associated with the role. The role names include a link to a page that allows you to manage the users and groups associated with the role. The page also includes a view of the data library datasets that are associated with the role and the permissions applied to each dataset.
    - **Job monitoring and management**
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    - **Install tools from the Tool Shed**
    - **Core facility sample tracking**
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# Galaxy Admin Interface



These features are only available once you define admin\_users!

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# A few more options

- Enable browsers like UCSC, GBrowse and **Galaxy Trackster**
  - `ucsc_display_sites`, `gbrowse_display_sites`, `enable_tracks`
- “sudo” for Galaxy: `allow_user_impersonation`
- Publishing features: `enable_pages`
- Disk quotas: `enable_quotas`

# Get a real database

- SQLite is serverless
- Galaxy is a heavy database consumer
- Locking will be an immediate issue
- Consumes Galaxy server process resources
- Migrating data is no fun
- Setup is very easy:  
`database_connection = postgres://`

PostgreSQL



```
victory# apt-get install postgresql
```

```
Reading package lists... Done
```

```
Building dependency tree
```

```
Reading state information... Done
```

```
The following extra packages will be installed:
```

```
libpq5 postgresql-9.1 postgresql-client-9.1 postgresql-client-common  
postgresql-common
```

```
Suggested packages:
```

```
oidentd ident-server locales-all postgresql-doc-9.1
```

```
The following NEW packages will be installed:
```

```
libpq5 postgresql postgresql-9.1 postgresql-client-9.1 postgresql-client-  
common postgresql-common
```

```
0 upgraded, 6 newly installed, 0 to remove and 0 not upgraded.
```

```
Need to get 0 B/8,951 kB of archives.
```

```
After this operation, 22.6 MB of additional disk space will be used.
```

```
Do you want to continue [Y/n]? Y
```

```
... magic happens ...
```

```
victory# su - postgres
```

```
postgres@victory:~$ createuser -SDR galaxy
```

```
postgres@victory:~$ createdb -O galaxy galaxy
```

```
postgres@victory:~$
```

# Offload the menial tasks: Proxy

- Directly serve static content faster than Galaxy's HTTP server
- Reduce load on the application
- Caching and compression
- Load balancing (more on that later)
- Hook your local authentication and authorization system

NGINX

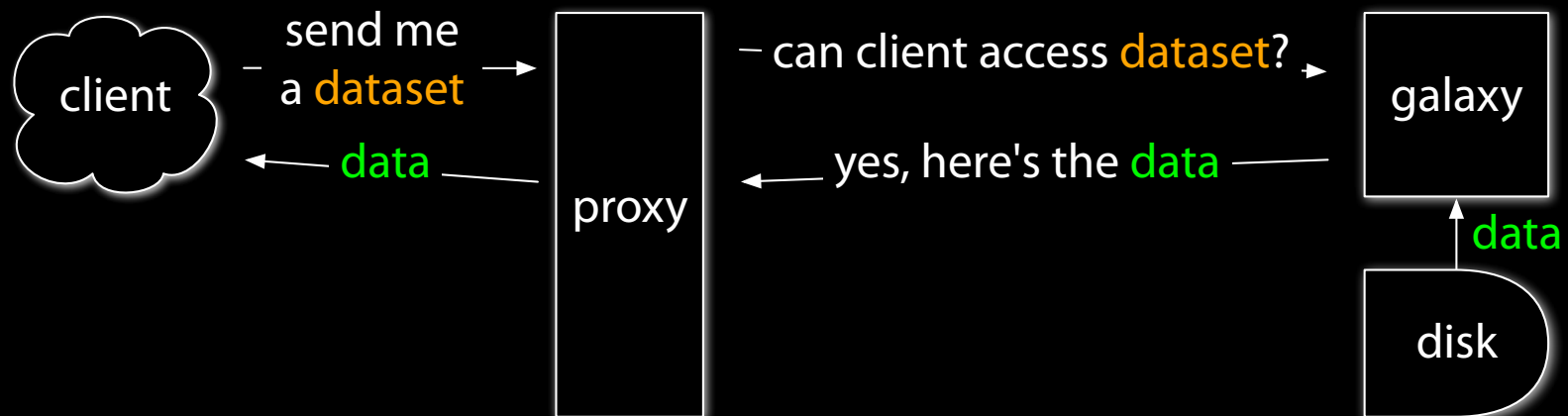


# Proxy Options

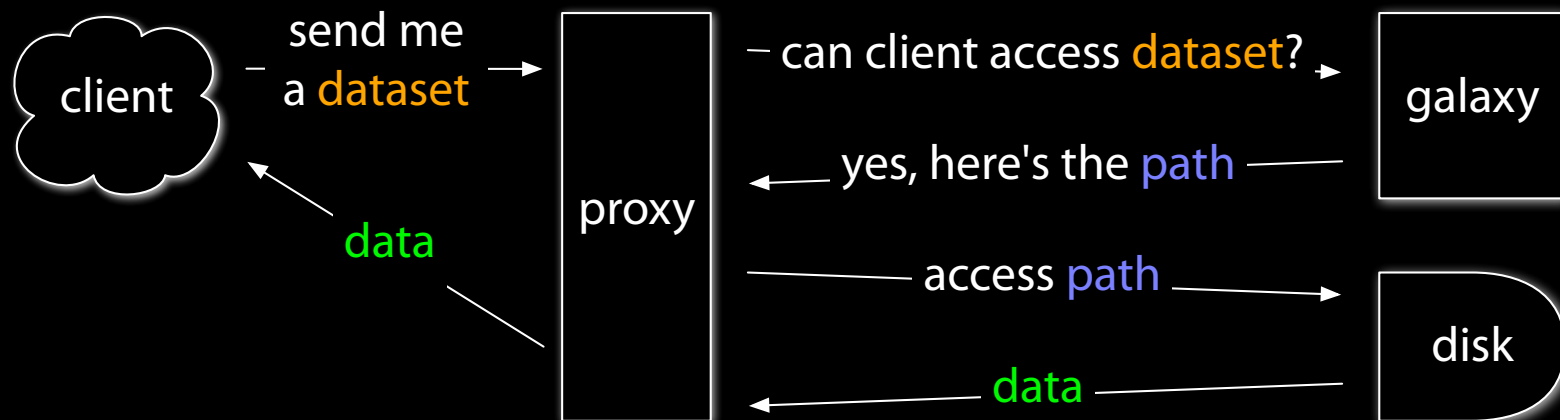
- Server
  - nginx
    - Designed with proxy as the primary purpose
    - Has an upload module
    - The proxy used for usegalaxy.org and Cloud Galaxy
  - Apache
    - More authentication and other 3rd party modules



# Downloading data from Galaxy



# Downloading data from the proxy

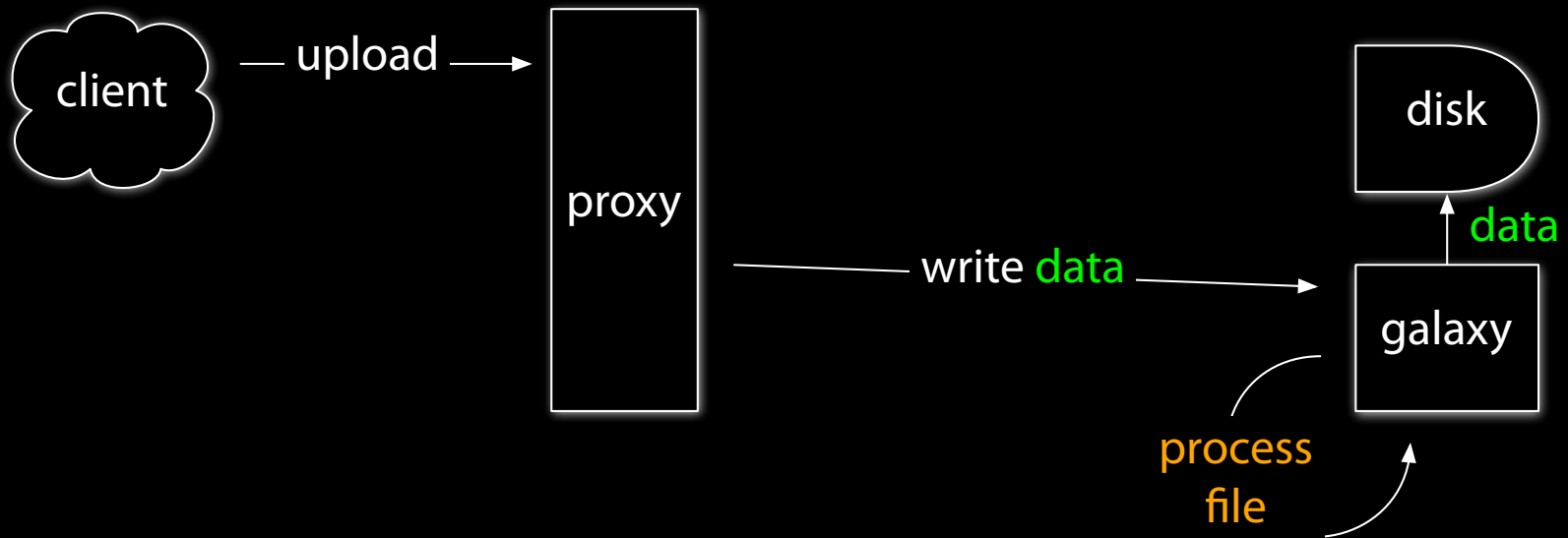


# Downloading data

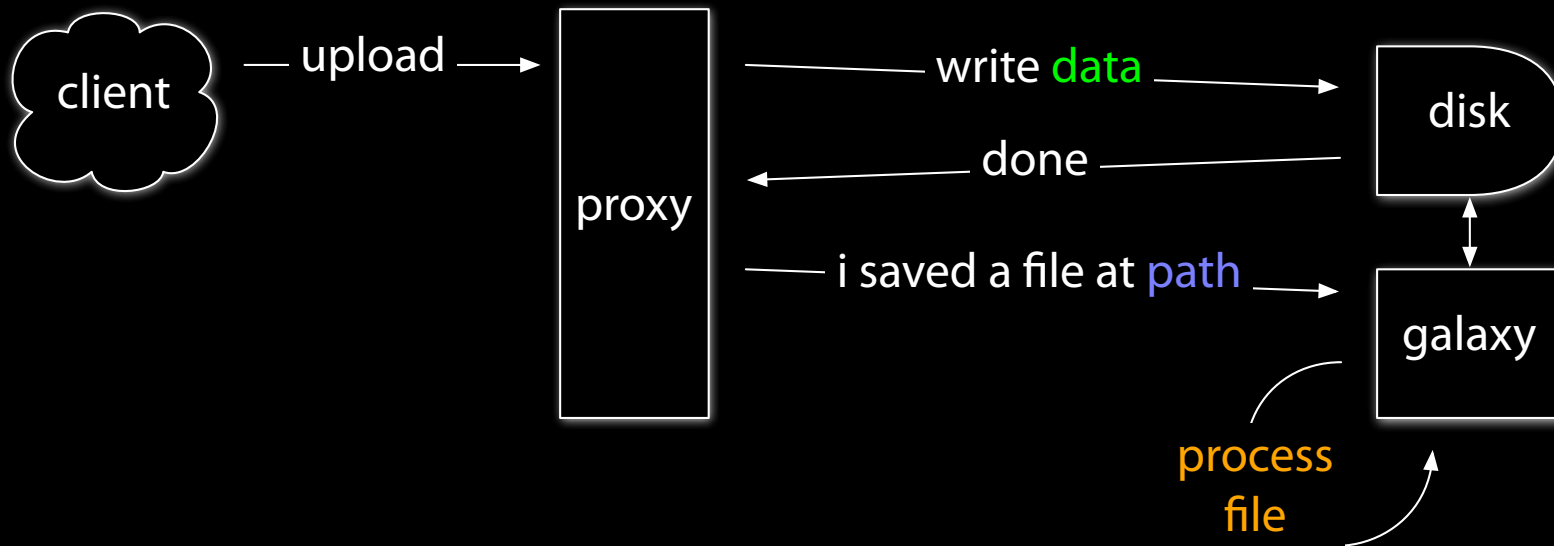
## from the proxy

- The proxy server can send files much faster than Galaxy's internal HTTP server and file I/O methods
- Reduce load on the application, free the process
- Restartability
- Security is maintained: the proxy consults Galaxy for authZ
- Proxy server requires minimal config and then:
  - nginx: `nginx_x_accel_redirect_base = /_download`
  - Apache: `apache_xsendfile = True`

# Uploading data to Galaxy



# Uploading data to the proxy (nginx)



# Uploading data

## to the proxy

- The proxy is also better at receiving files than Galaxy
- Again, reduce load on the application, free the process
- Again, restartability
- More reliable
- Slightly more complicated to set up, and nginx only

# Uploading data

## from a local filesystem

- Many browsers have file size limitations
- Interrupted uploads cannot be resumed
- You may want to upload directly from a server
- Perhaps your data is already on a filesystem locally accessible to the Galaxy server

# Uploading data

from a local filesystem

- For data libraries
- For histories



# Uploading data

## from a local filesystem

- Non-admin users may also upload to libraries from the local filesystem if granted permission and `user_library_import_dir` is set

# Uploading data

via FTP

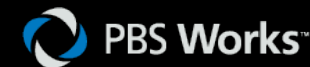
- FTP not explicitly required, cp, scp, sftp, whatever method your users have to place data on the server
- Full config example for ProFTPd with user authentication against Galaxy available in Wiki

# Caching data locally

- Some data (e.g. sequences and associated indexes) are useful to many but should automatically be recognized as available by tools
- Placing in a data library and requiring history import every time would be a nuisance
- Avoid duplication and wasted time repeatedly building indexes on the same sequences
- Manage locally cached data in Galaxy

# Limitless tool resources: Use a cluster (or two)

- Move intensive processing (tool execution) to other hosts
- Utilize existing resources
- No job interruption upon restart
- Per-tool cluster options
- DRMAA supports most other DRMs
- It's easy: Set `start_job_runners` and `default_cluster_job_runner` and go!



# Per-tool Job Control

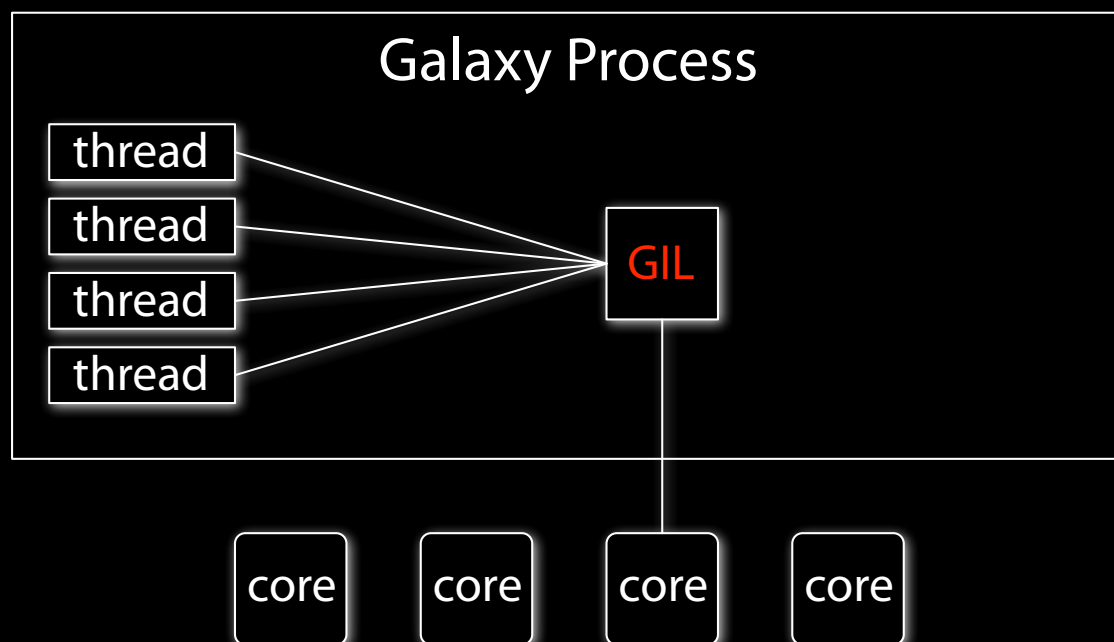
- `default_cluster_job_runner = pbs:///`
- `fastq_groomer = pbs://othercluster.example.org/groomerq`
- `bowtie_wrapper = pbs:///ngsq/-l nodes=1:ppn=8/`

# Job users on the cluster

- By default, jobs run as the user Galaxy is started as
- If your Galaxy users and cluster system users are identical, you may wish to run jobs on the cluster as the actual user
- Galaxy uses `sudo` to change ownership of relevant files and submit the job to the cluster as the correct system user
- Configurable for your specific environment

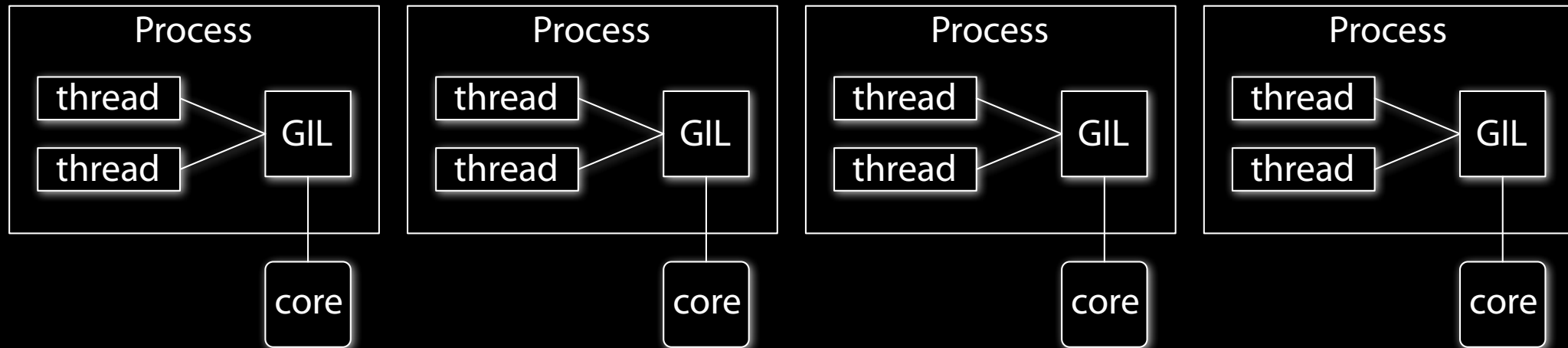
# Python and threading

- Galaxy is multi-threaded. No problem, right?
- Problem... Enter the Global Interpreter Lock



- Guido says: "run multiple processes instead of threads!"

# Opening the bottleneck



- One job manager - responsible for dispatching jobs to handlers
- Many job handlers - responsible for preparing and finishing jobs, monitoring cluster queue(s)
- Many web servers



# Defining extra servers is easy

```
[server:web_0]  
port = 8000  
[server:web_1]  
port = 8001  
[server:web_2]  
port = 8002  
...
```

```
[server:manager]  
port = 8099  
  
[server:handler0]  
port = 8100  
[server:handler1]  
port = 8101  
...
```

# Unload the Galaxy server

- Setting metadata is CPU intensive and will make Galaxy unresponsive
  - Make a new process (better yet, run on the cluster!)
  - All you need is: `set_metadata_externally = True`
- Run the data source tools on the cluster if they have access to the Internet
  - Remove `tool = local:///` from config file

# Data Management

- The Galaxy philosophy
  - Data is never overwritten
  - Data is never deleted

# Data Management

## filesystem choices

- Storage can easily be the bottleneck
  - Your storage must scale with your cluster
- Transparent compression and deduplication can reduce usage drastically
- Suggestions
  - ZFS: usegalaxy.org relies on ZFS on Solaris
  - ZFS on FreeBSD stable, Native ZFS on Linux coming
  - Btrfs may be viable soon

# Data Management

## creating data

- By default, all Galaxy history and library datasets are assigned an ID and stored in `galaxy-dist/database/files/`
- Single directory = single massive filesystem
- Galaxy has a dataset abstraction layer to decouple from a single local filesystem: Object Store
  - Disk backend: single filesystem
  - Distributed backend: multiple filesystems
  - Amazon S3 backend in development

# Data Management

creating data

```
object_store = distributed
```

```
<?xml version="1.0"?>  
<backends maxpctfull="90">  
  <backend id="pool1" type="disk" weight="5">  
    <files_dir path="/pool/pool1/files"/>  
    <extra_dir type="temp" path="/pool/pool1/tmp"/>  
    <extra_dir type="job_work" path="/pool/pool1/work"/>  
  </backend>  
  <backend id="pool2" type="disk" weight="1">  
    <files_dir path="/pool/pool2/files"/>  
    <extra_dir type="temp" path="/pool/pool2/tmp"/>  
    <extra_dir type="job_work" path="/pool/pool2/work"/>  
  </backend>  
</backends>
```

# Data Management

## cleaning data

- Data is never removed from disk unless
  - `allow_user_dataset_purge = True`
  - users click “delete permanently”
- Solution: `cleanup_datasets.py`
  - Run from cron to remove data from disk that has been deleted by the user (but not “deleted permanently”)
  - Configurable deletion policy allows removal after data has been deleted for a specified number of days

# Monitoring

- Monitor Galaxy
  - Provided methods:
    - With cron/email using `galaxy-dist/cron/check_galaxy.sh`
    - With Nagios using `galaxy-dist/contrib/nagios`
  - The provided scripts upload files and run jobs



# Collecting Statistics

- The Galaxy Reports webapp
  - Modify `galaxy-dist/reports_wsgi.ini` for your environment
  - Start the webapp with `sh run_reports.sh`

# Collecting Statistics

Galaxy Reports

https://admin.bx.psu.edu/galaxy/main/reports/

## 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

### All Jobs for May 2012

Click Total Jobs to see jobs for that day

Day	Date	User Jobs	Monitor Jobs	Total Jobs
Saturday	May 26, 2012	1115	155	<a href="#">1270</a>
Friday	May 25, 2012	5138	193	<a href="#">5331</a>
Thursday	May 24, 2012	4600	153	<a href="#">4753</a>
Wednesday	May 23, 2012	4384	188	<a href="#">4572</a>
Tuesday	May 22, 2012	5852	195	<a href="#">6047</a>
Monday	May 21, 2012	3905	198	<a href="#">4103</a>
Sunday	May 20, 2012	1423	193	<a href="#">1616</a>
Saturday	May 19, 2012	1158	182	<a href="#">1340</a>
Friday	May 18, 2012	4546	190	<a href="#">4736</a>
Thursday	May 17, 2012	4679	199	<a href="#">4878</a>
Wednesday	May 16, 2012	7378	185	<a href="#">7563</a>
Tuesday	May 15, 2012	5962	200	<a href="#">6162</a>
Monday	May 14, 2012	4803	179	<a href="#">4982</a>
Sunday	May 13, 2012	1563	196	<a href="#">1759</a>
Saturday	May 12, 2012	1555	151	<a href="#">1706</a>
Friday	May 11, 2012	5778	57	<a href="#">5835</a>
Thursday	May 10, 2012	4506	0	<a href="#">4506</a>
Wednesday	May 09, 2012	4812	0	<a href="#">4812</a>
Tuesday	May 08, 2012	5172	0	<a href="#">5172</a>



[usegalaxy.org/production](http://usegalaxy.org/production)

# The Team