A curated Domain centric shared Docker registry linked to the Galaxy toolshed
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A curated Domain centric shared Docker registry linked to the Galaxy toolshed

François Moreeews¹, Olivier Sallou², Yvan le Bras², Marie Grosjean³, Cyril Monjeaud², Thomas Darde⁴, Olivier Collin², Christophe Blanchet³

1 Genscale team -IRISA -Rennes, France
2 Genouest Bioinformatics facility – INRIA/IRISA – Rennes, France
3 French Institute of Bioinformatics – CNRS IFB-Core UMS3601 – Gif-sur-Yvette, France
4 INSERM U625 – Rennes France
“**Docker** is an open-source engine to easily create **lightweight, portable, self-sufficient containers** from any application. The same container that a developer **builds** and **test** on a laptop can run at **scale**, in **production**, on Vms,[...], public **clouds** and more.”
Why using Docker containers to build, deploy and execute applications?

- **Efficient** (no virtualization)
- **Isolation**
- **Build one time, execute “anywhere”, independently of the execution platform (laptops, clusters and clouds with Linux kernels)**

...
FROM ubuntu:12.0.4
ADD . /script
ENTRYPOINT ["perl /script/analysis.pl"]
Run Docker

docker -run
  containerUniqueID
  -k=31 -i input.fastq -o output.bam

-The docker run command acts as a wrapper of the tool command line.

-Host directories (input, output, work...) can be mounted inside the container.
Google Container Engine

- A container based cloud architecture
- “With container-based computing, application developers can focus on their application code, instead of on deployments and integration into hosting environments”.

Docker on the commercial Cloud
Docker on academic HPC clusters

- **Google Kubernetes**: an open source technology for containers life cycle management.
- **Docker Swarm**: allows to create and access to a pool of Docker hosts.
- **Genouest GO-DOCKER**: a batch scheduler like SGE, submitting jobs in Docker containers on top of Swarm.
Bioinformatics tools benchmarks with Docker

- cami-challenge.org: Critical Assessment of **Metagenomic** Interpretation
- http://nucleotid.es: continuous, objective and reproducible evaluation of genome **assemblers** using docker containers
- bioboxes.org: **interchangable** bioinformatics software containers
Galaxy Docker integration

- Docker can be used in Galaxy to:
  - manage tools dependencies: one tool, on Docker
  - Distribute populated Galaxy Distribution related to one topic
Shared registries: Docker Hub

• Not structured
• Not curated
• Not domain centric
• Not community driven
Shared registries : BIOSHADOCK

BIOSHADOCK

An initiative of the French Bioinformatics Institut & the Genouest Bioinformatics Facility

Goals :

• Federate bioinformatics tools deployment procedures for the IFB cloud infrastructure

• Generate customized Galaxy cloud instances on the fly.

• Docker image indexation (service registry & searches)
BioShaDock is a Bioinformatics Docker registry. Here are hosted Docker images dedicated to a broad spectrum of Biological communities as represented by the Biogenouest Western France network. In particular, you will find here:

- Command line tools;
- Complex web server frameworks;
- Galaxy Docker images that you can use with specific Docker Galaxy tools thanks to recent developments through the e-Biogenouest project (https://www.e-biogenouest.org/), (see GUGGO and our Toolshed);

The number of images available will grow following the community needs.

The Docker GenQuest core facility team:
François Moreews, Cyril Monjeaud, Yvan Le Bras, Olivier Sallou
**Shared registries : BIOSHADOCK**

### Images

<table>
<thead>
<tr>
<th>Images (34/34)</th>
</tr>
</thead>
<tbody>
<tr>
<td>abyss</td>
</tr>
<tr>
<td>bio-linux</td>
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<tr>
<td>bijava</td>
</tr>
<tr>
<td>bioperl</td>
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<tr>
<td>biopython</td>
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<tr>
<td>blast</td>
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<tr>
<td>bowtie</td>
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<td>bwa</td>
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<tr>
<td>centos</td>
</tr>
<tr>
<td>centos7</td>
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<tr>
<td>chado_database</td>
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<tr>
<td>clustal-omega</td>
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<tr>
<td>comet</td>
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<tr>
<td>discoasp</td>
</tr>
<tr>
<td>emboss</td>
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<tr>
<td>idba</td>
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<tr>
<td>ipython-notebook</td>
</tr>
<tr>
<td>imragist</td>
</tr>
<tr>
<td>minia</td>
</tr>
</tbody>
</table>

### Details for tag `library / stacks_galaxy : latest`

**Want to use this image?**

```bash
# Pull command:

docker pull docker-registry.genouest.org/stacks_galaxy:latest
```

**Run test command:**

```bash
docker run -l docker-registry.genouest.org/stacks_galaxy/latest /bin/bash
```

**Remark:** If the Docker client generates an SSL certificate error, you can solve this issue by adding an option `--insecure-registry docker-registry.genouest.org` in the Docker daemon command line. Modify the Docker daemon command line adding the following option:

```bash
DOCKER_OPTS="--insecure-registry docker-registry.genouest.org"
```

To do this on Ubuntu, modify `/etc/init/docker.conf`; on Debian, modify `/etc/init.d/docker`. Do not forget to restart the service: (`service docker restart`)

### Image Details

<table>
<thead>
<tr>
<th>General Information</th>
<th>Image Ancestry</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>Author</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Comment</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Created</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Docker version</strong></td>
</tr>
</tbody>
</table>
Shared registries: BIOSHADOCK

- BIOSHADOCK
  - Focuses on the model “on tool, one docker image”
  - Allows Dockerfile build
  - Manages permissions (private/public images)
  - May integrate meta data to facilitate query and service registry searches
  - One unique repository for softwares with or without tool.xml => SAAS + CMD
  - Integrated to Galaxy by redefining tools dependencies in a Toolshed
# BIOSHADOCK TOOLSHED integration

## Galaxy Tool Shed

- 164 valid tools on Jul 06, 2015

### Search
- Search for valid tools
- Search for workflows

### Valid Galaxy Utilities
- Tools
- Custom datatypes
- Repository dependency definitions
- Tool dependency definitions

### All Repositories
- Browse by category

### Available Actions
- Login to create a repository

### Repositories by Category

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alignment</td>
<td>Alignment tools</td>
</tr>
<tr>
<td>Data management</td>
<td>Tools for data management</td>
</tr>
<tr>
<td>Data manager</td>
<td>Biological data management</td>
</tr>
<tr>
<td>Data source</td>
<td>data source</td>
</tr>
<tr>
<td>Fasta / Fastq manipulation</td>
<td>Fasta / Fastq manipulation</td>
</tr>
<tr>
<td>France Genomique Assembly</td>
<td>Tools for NGS assembly as part of France Genomique Project</td>
</tr>
<tr>
<td>Metadata management</td>
<td>Tools for ISA manipulation</td>
</tr>
<tr>
<td>Metagenomics</td>
<td>NGS metagenomics analysis tools</td>
</tr>
<tr>
<td>Microarray</td>
<td>Analyse gene expression data through microarray technology</td>
</tr>
<tr>
<td>Next Generation Sequencing</td>
<td>NGS analysis tools</td>
</tr>
<tr>
<td>Phylogeny</td>
<td>phylogeny tools</td>
</tr>
</tbody>
</table>
Build it one time, use it as you want

Galaxy tools & workflows

BIOSHADOCK

Command lines

Other SAAS tools
References

- Genouest GO-DOCKER : http://www.genouest.org/?p=246
- Google Kubernetes, Docker container cluster management : kubernetes.io
- BioShaDock, a Bioinformatics Shared Docker registry : http://docker-ui.genouest.org
- GUGGO Galaxy Tooshed : http://toolshed.genouest.org
- Nucleotid.es, continuous, objective and reproducible evaluation of genome assemblers using docker containers : http://nucleotid.es
- ELIXIR Tools and Data Services Registry : https://elixir-registry.cbs.dtu.dk
- Bioboxes, a standard for creating interchangable bioinformatics software containers : http://bioboxes.org
- IFB academic Cloud : http://www.france-bioinformatique.fr/?q=en/core/e-infrastructure-team/ifb-cloud