CyVerse Documentation

CyVerse

Sep 18, 2020

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Tool integration in CyVerse Discovery Environment can be done either for executable tool (includes osg) or interactive tool.

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CHAPTER 1

OSG Tool Integration in DE

1.1 Goal

This quickstart contains the complete instructions for integrating OpenScienceGrid tools in CyVerse Discovery Environment. OSG tools are intended for high-throughput processing of many files.

1.2 Prerequisites

1.2.1 Downloads, access, and services

In order to complete this tutorial you will need access to the following services/software

Prerequisite	Preparation/Notes	Link/Download
CyVerse account	You will need a CyVerse account to complete this exercise	
Atmosphere Access (Optional – for building containers remotely)	Atmosphere access is by request only	Check or request access: CyVerse User Portal
Installation of Docker	Docker on the machine you're building containers	Atmosphere Installation instructions
Installation of Singularity	Singularity on the machine you're building containers	Atmosphere Installation instructions

1.2.2 Platform(s)

We will use the following CyVerse platform(s):

Platform	Interface	Link	Platform Documentation	Quick Start
Discovery Environment	Web/Point-and-click			
Atmosphere	Cloud Virtual Machine			

1.2.3 Input and example data

In order to complete this quickstart you will need to have the following inputs prepared

Input File(s)	Format	Preparation/Notes	Example Data
Read1.fastq	fastq	Make sure it is a fastq file and not fasta file	Read1.fastq

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1.3 Get started

- Create a Docker image for your tool/software of interest
- Build the Docker image for your tool/software
- Test Docker image
- Submit a pull request to OSG github repo
- Integrate DE tool using "Add Tools" option in DE

1.3.1 1. Create a Docker image for your tool

This is the first step in the process of making OSG tool integration in DE. The minimum requirements for creating a Docker image include the following dependencies (apart from the dependencies that are needed for your tool of interest)

Operating System	Directories	Dependencies	Files
Debian	`/work`	`icommands`	`wrapper`
Ubuntu 16+	`/cvmfs`	`wget`	`upload-files`
Centos7+		`python3`	`create-ticket.sh`

For this example, we will use fastq-sample.

Let's first create a Dockerfile using your favorite editor which satisfies the above requirements

```
$ mkdir fastq-sample-osg && cd fastq-sample-osg

$ wget https://data.cyverse.org/dav-anon/iplant/projects/osg/upload-files

$ wget https://data.cyverse.org/dav-anon/iplant/projects/osg/wrapper
```

```
$ vi Dockerfile

FROM ubuntu:xenial
MAINTAINER User Name <user@cyverse.org>
```

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```
RUN mkdir /cvmfs /work

RUN apt-get update \
    && apt-get install -y lsb curl apt-transport-https python3 python-requests␣
↪libfuse2 wget gcc make libpcre3-dev libz-dev

# Install fastq-tools
RUN wget http://homes.cs.washington.edu/~dcjones/fastq-tools/fastq-tools-0.8.tar.gz
RUN tar xvf fastq-tools-0.8.tar.gz
WORKDIR fastq-tools-0.8
RUN ./configure
RUN  make install fastq==0.8

WORKDIR /work

# Define the iRODS package
ENV ICMD_BASE="https://files.renci.org/pub/irods/releases/4.1.12/ubuntu14"
ENV ICMD_PKG="irods-icommands-4.1.12-ubuntu14-x86_64.deb"

# Install icommands.
RUN curl -o "$ICMD_PKG" "$ICMD_BASE/$ICMD_PKG" \
        && dpkg -i "$ICMD_PKG" \
        && rm -f "$ICMD_PKG"

# Install the wrapper script and the script to upload the output files.
ADD wrapper /usr/bin/wrapper
ADD upload-files /usr/bin/upload-files

# Make the wrapper script the default command.
CMD ["wrapper"]
```

Note: The `Dockerfile` and `wrapper` files are specific for this example `fastq-sample` tool.

If you want to create OSG tool for your tool of interest, replace the specific parts of the script

in `wrapper` script append lines # 117-122 with your job information:

```
   # Run the job.
def run_job(arguments, output_filename, error_filename):
    with open(output_filename, "w") as out, open(error_filename, "w") as err:
        rc = subprocess.call(["fastq-sample"] + arguments, stdout=out, stderr=err)
        if rc != 0:
            raise Exception("fastq-sample returned exit code {0}".format(rc))
```

Note: Be sure the `upload-files` and `wrapper` scripts are executable. This can be done by adding the following line to your Dockerfile:

```
# Make scripts executable:
RUN chmod +x /usr/bin/upload-files /usr/bin/wrapper
```

1.3.2 2. Build and push the Docker image to Dockerhub

Once you create the Dockerfile, next step is to build the Docker image and push it to Dockerhub manually (you can also do an automated build)

```
$ docker build -t upendradevisetty/fastq-sample-osg:0.8 .

$ docker push upendradevisetty/fastq-sample-osg:0.8
```

1.3.3 3. Test Docker image

Testing of OSG-fastq-sample docker image can be done in two ways: Locally using Singularity and on Open Science Grid (OSG). Since many users don't have access to OSG, we recommed that you test it locally.

Important: This is very important step as it is very hard to troubleshoot after you integrate the OSG tool in DE

3.1 Create a folder with input file(s) and output folder on CyVerse Datastore

For this example, the only input file is *Read1.fastq*. I have this input file in this path on Datastore */iplant/home/upendra_35/fastq-sample-osg/Read1.fastq* and output folder in this path on Datastore */iplant/home/upendra_35/fastq-sample-osg/output*

3.2 Create input and output path files

The next step is to create an input and output path files that contains the paths to the input and output respectively.

```
$ cat input-paths.txt
  /iplant/home/upendra_35/fastq-sample-osg/Read1.fastq

$ cat output-paths.txt
  /iplant/home/upendra_35/fastq-sample-osg/output
```

3.3 Create input and output tickets from input and output paths files

Using *create-tickets.sh <https://github.com/upendrak/fastq-sample-osg/blob/master/create-tickets.sh>*, create tickets for both inputs and outputs

```
$ wget https://raw.githubusercontent.com/upendrak/fastq-sample-osg/master/create-
↪tickets.sh

$ mkdir sample_data

$ bash create-tickets.sh -r input-paths.txt > sample_data/input_ticket.list
$ cat sample_data/input_ticket.list
  # application/vnd.de.path-list+csv; version=1
  c0837571b6b7416fb998c5b9b226ea,/iplant/home/upendra_35/fastq-sample-osg/Read1.fastq

$ bash create-tickets.sh -w output-paths.txt > sample_data/output_ticket.list
$ cat sample_data/output_ticket.list
  # application/vnd.de.path-list+csv; version=1
  3fe4ea0dab5241cfb69420335c0902,/iplant/home/upendra_35/fastq-sample-osg/output
```

3.4 Create a `config.json` file in the `sample_data` folder

Here is an example of `config.json` for the `fastq-sample-osg` tool

```
$ vi sample_data/config.json
 {
     "arguments": [
         "-n",
         "10",
   "Read1.fastq"
     ],
     "irods_host": "davos.cyverse.org",
     "irods_port": 1247,
     "irods_job_user": "upendra_35",
     "irods_user_name": "job",
     "irods_zone_name": "",
     "input_ticket_list": "input_ticket.list",
     "output_ticket_list": "output_ticket.list",
     "status_update_url": "https://de.cyverse.org/job/bd1a1b53-9a7e-4031-bf0c-
↪227a0c63f555/status",
     "stdout": "out.txt",
     "stderr": "err.txt"
 }
```

This is similar to running on the commandline like this..

```
$ fastq-sample -n 10 Read1.fastq
```

3.5 Pull the Docker image as singularity file (.sif)

Important: You must have Singularity installed to complete this step.

```
$ singularity pull docker://upendradevisetty/fastq-sample-osg:0.8
```

This will create *fastq-sample-osg_0.8.sif* singularity image in your working directory

3.6 Test the singularity image

Important: Remove your current iRODS password: `rm ~/.irods/.irodsA`

Running this container will overwrite the `~/.irods/irods_environment.json` file on the localhost. To re-generate the previous iRODS environment, `rm -rf ~/.irods/irods_environment.json` and run `iinit` again.

Once you have created the `input_ticket.list`, `output_ticket.list` and `config.json` files in the `/sample_data` directory, you are ready for a test with the Singularity image:

```
$ cd sample_data

$ singularity exec ../fastq-sample-osg_0.8.sif ../wrapper
  running: configuration successfully loaded
  running: initializing the iRODS connection
  running: downloading the input files
  Enter your current iRODS password:
  running: processing the input files
  running: uploading the output files
  Enter your current iRODS password:
  Enter your current iRODS password:Enter your current iRODS password:
```

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```
Enter your current iRODS password:
Enter your current iRODS password:
Enter your current iRODS password:Enter your current iRODS password:
Enter your current iRODS password:Enter your current iRODS password:completed: job␣
↪completed successfully
```

Note: It will prompt you to enter your irods passwords several times, if so, then keep pressing the ENTER until the job is successfully finished. The output files will be uploaded to your output folder in datastore.

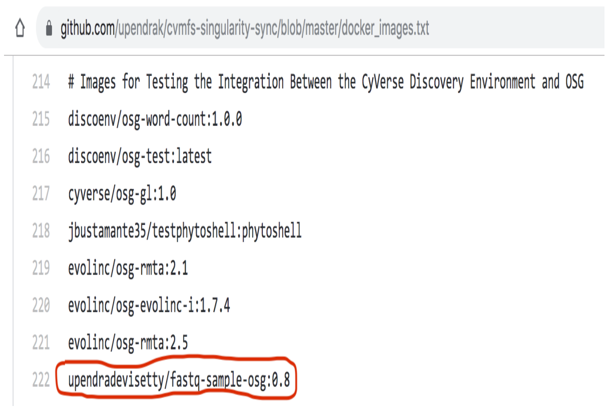
Once your job has finished, you should expect to see the input (`Read1.fastq`) and output (`sample.fastq`) files in the current working directory and also in the in the output directory.

1.3.4 4. Submit a pull request to OSG github repo for `fastq-sample-osg` tool

Once the Singularity run works, add your Docker image in here. For this particular example, we will add `upendradevisetty/fastq-sample-osg:0.8` in there.

Note: You will have to fork and do a PR for this to work

Here is a screenshot of `fastq-sample-osg:0.8` pull request to OSG github repo



github.com/upendrak/cvmfs-singularity-sync/blob/master/docker_images.txt

```
# Images for Testing the Integration Between the CyVerse Discovery Environment and OSG
discoenv/osg-word-count:1.0.0
discoenv/osg-test:latest
cyverse/osg-gl:1.0
jbustamante35/testphytoshell:phytoshell
evolinc/osg-rmta:2.1
evolinc/osg-evolinc-i:1.7.4
evolinc/osg-rmta:2.5
upendradevisetty/fastq-sample-osg:0.8
```

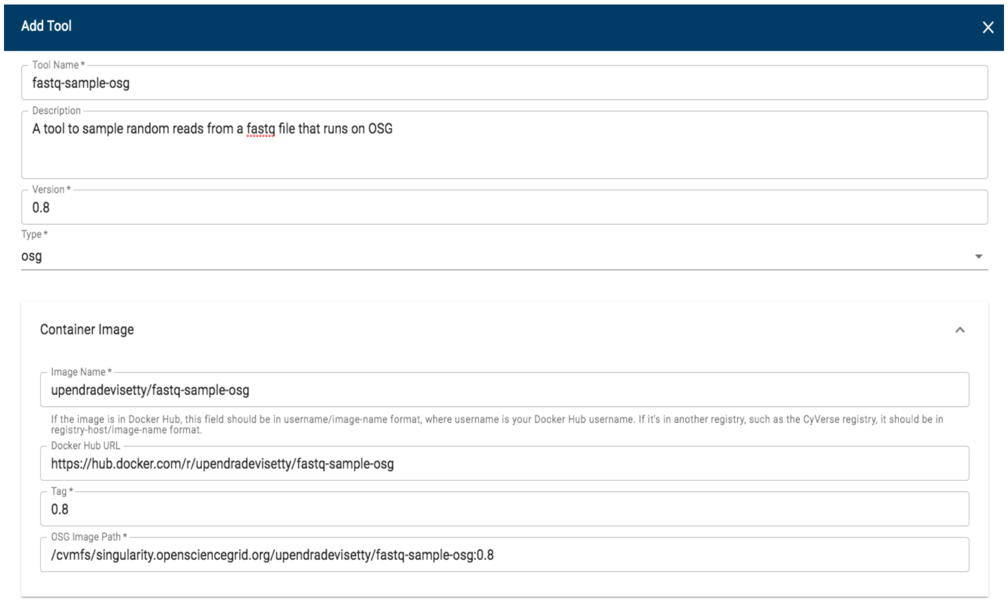
After the PR is merged, it takes few hours for the image to be available on CVMFS.

1.3.5 5. Integrate DE tool using “Add Tools” option in DE

After the image is available on OSG, it is now ready to be integrated into DE.

5.1 Log-in to CyVerse Discovery Environment and click on the “Apps” window

5.2 Click “Manage Tools” -> “Tools” -> “Add Tool” and fill the details about your Docker image



Tool Name *
fastq-sample-osg

Description
A tool to sample random reads from a fastq file that runs on OSG

Version *
0.8

Type *
osg

Container Image

Image Name *
upendradevisetty/fastq-sample-osg

If the image is in Docker Hub, this field should be in username/image-name format, where username is your Docker Hub username. If it's in another registry, such as the CyVerse registry, it should be in registry-host/image-name format.

Docker Hub URL
https://hub.docker.com/r/upendradevisetty/fastq-sample-osg

Tag *
0.8

OSG Image Path *
/cvmfs/singularity.opensciencegrid.org/upendradevisetty/fastq-sample-osg:0.8

Procede here to create an app interface in the CyVerse Discovery Environment

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1.3.6 Additional information, help

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CHAPTER 2

Interactive (VICE) Tool Integration in DE

2.1 Goal

This quickstart contains the complete instructions for integrating interactive (VICE) tools in DE which is mainly intended for exploratory data analysis (bioinformatic and geoinformatic) as well as the ability to run ad-hoc scripts.

Tip: What is interactive tool?

Any tool that needs to run on the web browser by opening up ports is considered as an interactive tool

For more information on Interactive tools, please refer to this extensive documentation

2.2 Prerequisites

2.2.1 Downloads, access, and services

In order to complete this tutorial you will need access to the following services/software

Prerequisite	Preparation/Notes	Link/Download
CyVerse account	You will need a CyVerse account to complete this exercise	

2.2.2 Platform(s)

We will use the following CyVerse platform(s):

Platform	Interface	Link	Platform Documentation	Quick Start
Discovery Environment	Web/Point-and-click			

2.3 Get started

- Find the Docker image of your interactive tool/software of your interest
- Test the Docker image
- Add the interactive tool in CyVerse Discovery Environment

1. Find the Docker image

We will use PEA-Rstudio, an integrated R toolkit for epitranscriptome analysis for integrating as an interactive tool in DE. Fortunately, there is Docker image available for *PEA* on Dockerhub for integrating that as an interactive tool in DE.

Note: If there is no Docker image available for your tool of interest, then you would either find a Dockerfile which you can use to build the Docker image for your tool of interest or create one. You can get more help with either of that from here

2. Test the Docker image locally on your computer (Optional but recommended)

This is optional but highly recommended step to confirm that the Docker image for your tool of interest is working as expected. Here is how you would test PEA with the intructions they provided in their README

2.1 Pull the image from Dockerhub

```
$ docker pull malab/pea:v1.1_rstudio
```

If you are looking for a place to pull the Docker image or run the Docker container, then you can use the free resource - Play with Docker

2.2 Sample run

Once PEA-Rstudio Docker image is pulled successfully, type the following command to start PEA

```
$ docker run --rm -d -p 8787:8787 malab/pea:v1.1_rstudio
```

Note: The username and password for Rstudio is `rstudio` and `pea` respectively

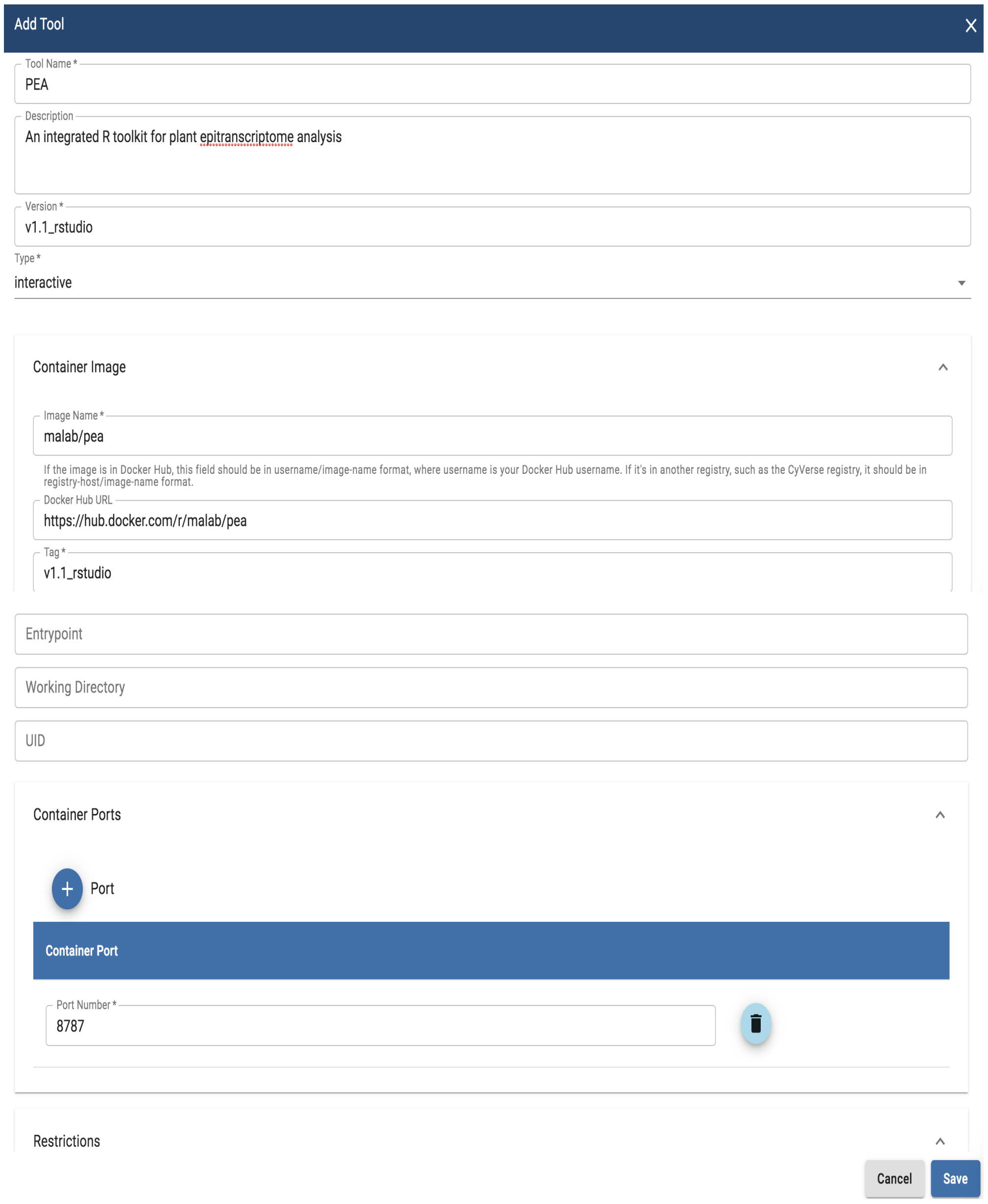
Once you can open the Rstudio, then you are ready to integrate the tool in DE

3. Add tool in CyVerse Discovery Environment

Now that the PEA-Rstudio Docker image has been tested, it is now ready to be integrated into DE.

3.1 Log-in to CyVerse Discovery Environment and click on the "Apps" window

3.2 Click "Manage Tools" -> "Tools" -> "Add Tool" and fill the details about your Docker image



Add Tool

Tool Name *
PEA

Description
An integrated R toolkit for plant epitranscriptome analysis

Version *
v1.1_rstudio

Type *
interactive

Container Image

Image Name *
malab/pea

If the image is in Docker Hub, this field should be in username/image-name format, where username is your Docker Hub username. If it's in another registry, such as the CyVerse registry, it should be in registry-host/image-name format.

Docker Hub URL
https://hub.docker.com/r/malab/pea

Tag *
v1.1_rstudio

Entrypoint

Working Directory

UID

Container Ports

Container Port

Port Number *
8787

Restrictions

Procede here to create an app interface in the CyVerse Discovery Environment

2.3.1 Additional information, help

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CHAPTER 3

Goal

This 3-step quickstart allows users to integrate the Docker images of their favorite software as **executable** tool type in DE. If users are interested in integrating the Docker images of their favorite software as **osg** or **interactive**, please refer to here and here respectively.

Important: What is executable software/tool?

Any software/tool that can be run on the command line without the need to open any ports

CHAPTER 4

Prerequisites

4.1 Downloads, access, and services

In order to complete this tutorial you will need access to the following services/software

Prerequisite	Preparation/Notes	Link/Download
CyVerse account	You will need a CyVerse account to complete this exercise	

4.2 Platform(s)

We will use the following CyVerse platform(s):

Platform	Interface	Link	Platform Documentation	Quick Start
Discovery Environment	Web/Point-and-click			

4.3 Input and example data

In order to complete this quickstart you will need to have the following inputs prepared

Input File(s)	Format	Preparation/Notes	Example Data
Read1.fastq	fastq	Make sure it is a fastq file and not fasta file	Read1.fastq

CHAPTER 5

Get started

- Find the Docker image of your tool/software of your interest
- Test the Docker image with the test data
- Add tool in CyVerse Discovery Environment

1. Find the Docker image

We will use fastq-sample for integrating as tool in DE. Fortunately, there is Docker image available for *fastq-sample* on Dockerhub and so we can use that fastq-sample docker image for integrating that as tool in DE.

Note: If there is no Docker image available for your tool of interest, then you would either find a Dockerfile which you can use to build the Docker image for your tool of interest or create one. You can get more help with either of that from here

2. Test the Docker image locally on your computer (Optional but recommended)

This is optional but highly recommended step to confirm that the Docker image for your tool of interest is working as expected. Here is how you would test fastq-sample with the intructions they provided in their README

2.1 Pull the image from Dockerhub

```
$ docker pull upendradevisetty/fastq-sample:0.8
```

2.2 See the command line help for the image

```
$ docker run upendradevisetty/fastq-sample:0.8 -h
  fastq-sample [OPTION]... FILE [FILE2]
  Sample random reads from a FASTQ file.Options:
  -n N                    the number of reads to sample (default: 10000)
  -p N                    the proportion of the total reads to sample
  -o, --output=PREFIX     output file prefix
 (Default: "sample")  -c, --complement-output=PREFIX
                          output reads not included in the random sample to
                          a file (or files) with the given prefix (by default,
```

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```
                             they are not output).
  -r, --with-replacement     sample with replacement
  -s, --seed=SEED            a manual seed to the random number generator
  -h, --help                 print this message
  -V, --version              output version information and exit
```

2.3 Sample run with an example file

```
$ docker run --rm -v $PWD:/data -w /data upendradevisetty/fastq-sample:0.8 -n 10␣
↪Read1.fastq
```

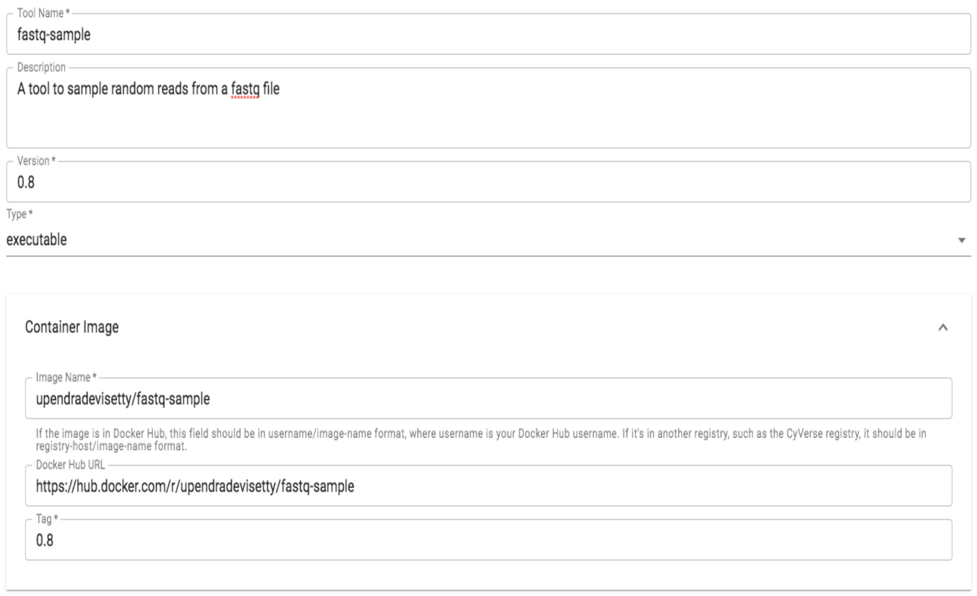
Once you get the expected output, then you are ready for the next step

3. Add tool in CyVerse Discovery Environment

Now that the *fastq-sample* Docker image has been tested, it is now ready to be integrated into DE.

3.1 Log-in to CyVerse Discovery Environment and click on the "Apps" window

3.2 Click "Manage Tools" -> "Tools" -> "Add Tool" and fill the details about your Docker image



Tool Name *
fastq-sample

Description
A tool to sample random reads from a fastq file

Version *
0.8

Type *
executable

Container Image

Image Name *
upendradevisetty/fastq-sample

If the image is in Docker Hub, this field should be in username/image-name format, where username is your Docker Hub username. If it's in another registry, such as the CyVerse registry, it should be in registry-host/image-name format.

Docker Hub URL
https://hub.docker.com/r/upendradevisetty/fastq-sample

Tag *
0.8

Procede here to create an app interface in the CyVerse Discovery Environment

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