

Quick Start: How to do some common tasks?

There are three terms you need to know about Docker:

Docker Image: A Docker template file, e.g. a standard Ubuntu Linux image;

Docker container: A running instance of the Docker image;

Shell of a container: A Linux shell to access a Docker container;

If you still do not know about the meaning of the terms, do not worry. They will start to make sense after some practices.

Task 1: Install the software in a Docker container, which can be saved in a new Docker image and used later.

- **Step 1.** Import a template Docker image. This step could take 1-3 minutes. I am using "Ubuntu" as an example here. The "docker1 images" command can be used to check images that have already been imported on your machine.

```
docker1 pull biohpc/ubuntu-dev
docker1 images
```

- **Step 2.** Start a Docker Container (an instance of the image). You need to replace "docker.io/biohpc/ubuntu-dev" in the example below with the actual image name on your machine. The "docker1 images" command would tell you the names of the available images. The "-d" option in this step is to make sure that the container will run in the background. Use the "docker1 ps -a" command to check containers that are currently running on your machine.

```
docker1 run -d -it docker.io/biohpc/ubuntu-dev /bin/bash
docker1 ps -a
```

- **Step 3.** Start an interactive shell to access the Docker Container. To do this, you need the container name, which is a string that looks like "d3b7d7463857". Replace d3b7d7463857 in this example with the actual container name. Use the "docker1 ps -a" command to get the container name. After Login, you might want to run update and upgrade to update all the packages

```
docker1 exec -it d3b7d7463857 /bin/bash
apt-get update
apt-get upgrade
```

- **Step 4.** After step 3, you are in an interactive shell of a Docker container. As you have root privilege here, you can install any software you like, /usr/bin. **Do not install software in /workdir in the Docker container**, as the /workdir in the Docker container is the directory for you to interact with the hosting system.
Sometime, a software could take a long time to install. If your internet connection got interrupted in the middle when installing a software. Do not worry, the container is still running in the background. You can start a new ssh session, and use the command "docker1 exec -it d3b7d7463857 /bin/bash" to access the same container.
- **Step 5.** As you might need to use the installed software several times later, you can save the container in a new Docker image, and keep that image in your home directory. To do this, first you need to exit the interactive shell, then use the "docker1 export" command. The saved image can be imported later with "docker1 import /home/qisun/myfile.tar". The image file for "Ubuntu Dev." is about 0.8GB.

```
exit  
docker1 export -o /home/qisun/myfile.tar d3b7d7463857
```

Task 2: Run the software in Docker.

- **Step 1.** Import the Docker image with the software you want to use. Before you do that, please use the "docker1 images" command to check whether the images you want to use is already on the machine. If not, use the "docker1 import <file>" command to import the image.

```
docker1 images  
docker1 import /home/qisun/myfile.tar
```

- **Step 2.** Start a Docker Container with the image. This step is the same as step 2 in task 1.

```
docker1 run -d -it biohpc_qisun/ubuntu-dev /bin/bash  
docker1 ps -a
```

- **Step 3.** Run the software. There are two alternative ways to run a Linux software in Docker.

1. Direct mode:

If the software does not take much time to finish,

```
docker1 exec d3b7d7463857 mycommand
```

If the software takes a long time to finish, you need to run it in background. For example:

```
docker1 exec d3b7d7463857 /bin/bash -c "bwa aln mydata >& log" &
```

To check whether a software is finished in Docker, use this command:

```
docker1 exec d3b7d7463857 ps -ef
```

2. Interactive mode with the "-it" option (This might be easier for some people)
Some software, e.g. "top", have to be run in an interactive mode. Use the following command to start an interactive shell. After this, you can type the command, e.g. top.

```
docker1 exec -it d3b7d7463857 /bin/bash
```

Some tips:

1. You can have multiple ssh sessions to access the same Docker container. Use "docker1 exec d3b7d7463857 mycommand" or "docker1 exec -it d3b7d7463857 /bin/bash" to connect to a Docker container.
2. If you reserve a machine from BioHPC Lab, the Docker containers and images will be deleted after the reservation end. If you want to re-use the container later, make sure to export the container to a new image file and save the new image in your home directory.
3. If something goes wrong, you can always remove the containers using the "docker1 clean" or "docker1 clean all" command. The "docker1 clean" remove the idle containers, which "docker1 clean all" remove all containers.