Using Docker in BioHPC Cloud

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Part 1 – presentation

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What is Docker?

A Linux subsystem to run isolated Linux "machines" called "containers"

Isolated means that programs, users and storage in Docker "machine" are separated from the host system.

It can run any flavor of Linux on any Linux machine – Docker container looks like a complete standalone Linux server with all files, programs and settings.

What is Docker?

Programs installed inside Docker container don't need to be compatible with the host, and in fact they need to be installed from scratch, regardless of what is installed on the host.

Regular user can become "root" (Linux administrator) inside Docker container, or any user as needed.

Docker components

image - a template than can be loaded into Docker and executed. Image can be stored on a disk as a file or in a specialized Docker repository of images

container - a running instance of Docker image – actual Docker "machine". Users can execute programs, install software and work in container as in a regular Linux system.

Docker components

image - like a program on the disk – it contains all information needed, but it needs to be loaded into memory to run.

container – like a program running on a computer – in the memory, can load data, change its own stored memory data etc.

Virtual Machine vs Docker Containers



Machine Virtualization

Virtual Machine (VM) is a separated "server" emulating its own hardware and running its own operating system. The only interaction with host OS is via hardware or emulated hardware.

VM can run any OS but is slower and requires extra resources to run. Up to 20-30% overhead.

Virtual Machine vs Docker Containers

Docker shares host OS kernel services and some libraries (readonly). It runs as a process in host operating system. It can access host files directly (optional).

No execution overhead – same speed. Cannot run non-Linux OS.



Docker security

In order to use original Docker user must have "root" access to certain parts of Linux OS.

It is safe for admins to deploy software, but NOT safe for users in multi-user environment like BioHPC

We have developed our own version of Docker on the top of original Docker that addresses security problems at the same time preserving most of Docker features.

Original Docker command is "docker". This command has been replaced by "docker1" command in BioHPC Lab.

Whenever reading a Docker book or website please replace "docker" with "docker1" when you want to run the command on BioHPC Lab machines.

If you run "docker" instead of "docker1" you will get an error. You have to use "docker1"

[jarekp@cbsum1c2b014 ~]\$ docker ps -a
Cannot connect to the Docker daemon. Is the docker daemon running on this host?
[jarekp@cbsum1c2b014 ~]\$

[jarekp@cbsum1c1b009 ~]\$ docker ps -a
Got permission denied while trying to connect to the Docker daemon socket at
unix:///var/run/docker.sock: Get
http://%2Fvar%2Frun%2Fdocker.sock/v1.26/containers/json?all=1: dial unix
/var/run/docker.sock: connect: permission denied

You can check docker1 options with "docker1 --help" or "docker1 commandname --help"

[jarekp@cbsum1c1b009 ~]\$ docker1 --help

This is BioHPC Cloud docker1 implementing secure Docker environment. Some Docker commands have been modified or disabled, but most are unchanged. There are three additional commands in docker1 listed below

clean Deletes sets of containers

claim Changes ownership of all files and dirs in /workdir/labid and /SSD/labid to labid white Displays set of options that are whitelisted to use with docker1 Special option --noworkdir for run command disables automatic mapping of /workdir and /SSD Please note you need to put docker command options BEFORE container name where applicable Docker help page follows.

Usage: docker COMMAND

A self-sufficient runtime for containers

Docker images

Before running any Dockerized application you need to know how to access its Docker image.

 Images are stored in Docker registries (or hubs) and their names and addresses are described in software documentation.
 docker1 pull docker.io/biohpc/imagename
 BioHPC image, public docker1 pull docker.io/imagename

General public image

 Image can be imported from a file docker1 load -i filename docker1 import filename

docker.io/ part may be omitted, repositories known to this Docker installation will be queried in order

Docker images: load vs import

docker1 load -i filename

Docker load command creates a container from saved image, it imports all the image layers, tags and settings. File for load command must be created with save command.

docker1 import filename
 Docker import command creates a container from saved
 container, it creates a simplified image based on the
 saved container with a single layer and no settings
 (like entry point). File for import command must be
 created with export command

To run a container:

- Pull or import/load image
- Start container from image

You can also start container without pulling first (only from registry, not a file), Docker will pull from hub it if not found locally. All images used on a server are cached in a local registry.

docker.io/ part may be omitted, repositories known to this Docker installation will be queried in order

Pull image

[jarekp@cbsum1c1b009 ~]\$ docker1 pull biohpc/cowsay Using default tag: latest Trying to pull repository dtr.cucloud.net/biohpc/cowsay ... Trying to pull repository docker.io/biohpc/cowsay ... sha256:c4c5c72fd2e09e35a02199aef774f5338ab6a17f204ed7317f11a58f8d1ad284: Pulling from docker.io/biohpc/cowsay 9e4b184d5239: Pull complete 4a28c3c49d95: Pull complete Digest: sha256:c4c5c72fd2e09e35a02199aef774f5338ab6a17f204ed7317f11a58f8d1ad284 Status: Downloaded newer image for docker.io/biohpc/cowsay:latest

[independent of hood]f	de else att dimense		List images	
[]arekp@cbsumicib009 ~]\$	docker1 1mages	5		
REPOSITORY	TAG	IMAGE ID	CREATED	SIZE
<pre>docker.io/biohpc/cowsay</pre>	latest	195f168235c9	3 years ago	337 MB
<pre>[jarekp@cbsum1c1b009 ~]\$</pre>				

cowsay is a **program** that generates ASCII pictures of a cow with a message. It can also generate pictures using pre-made images of other animals, such as Tux the Penguin, the Linux mascot. It is written in Perl. There is also a related **program** called cowthink, with cows with thought bubbles rather than speech bubbles.

en.wikipedia.org > wiki > Cowsay 💌

cowsay - Wikipedia



Import image

[jarekp@cbsum1c2b014 ~]\$ docker1 import /programs/docker/images/cowsay.tar sha256:da8e563445a8792ae5b161b446e8ef9ca2c76f2bafab58ad88bf0adcbfb5d0b0

<pre>[jarekp@cbsum1c2b014 ~]\$</pre>	docker1 images			
REPOSITORY	TAG	IMAGE ID	CREATED	SIZE
biohpc_jarekp/cowsay	latest	da8e563445a8	About a minute ago	319.7 MB
docker.io/biohpc/cowsay	latest	195f168235c9	16 months ago	337.1 MB
<pre>[jarekp@cbsum1c2b014 ~]\$</pre>				

What if we try to load a file created with export?

[jarekp@cbsumm15 docker]\$ docker1 load -i /programs/docker/images/cowsay.tar
open /local/docker/tmp/docker-import-755479071/dev/json: no such file or directory
[jarekp@cbsumm15 docker]\$

Run Docker container

• Single command

Run a command and then container stops.

• Interactive mode

Open shell inside container for interactive work. Once you are finished, exit shell and container stops.

Background mode

Start container in the background and connect to it when needed. Container will keep running.

Single command run

command image_name program program_arguments

[jarekp@cbsum1c2b014 ~]\$ docker1 run biohpc/cowsay cowsay "This is Docker"







[jarekp@cbsum1c2b014 ~]\$ docker1 exec 10af80003f76 cowsay "hi"

< hi > -----\ ^__^ \ (oo)____ (__)\ ||----w

Run in the background

```
[jarekp@cbsum1c2b014 ~]$ docker1 exec -it 10af80003f76 /bin/bash
[root@10af80003f76 ~]# ls -al
total 0
drwxr-xr-x 2 4965 root 6 May 22 17:26 .
drwxr-xr-x 18 root root 288 May 22 18:48 ..
[root@10af80003f76 ~]# exit
exit
```

[jarekp@cbsum1c2b014 ~]\$ docker1 ps -a

CONTAINER IDIMAGE10af80003f76biohpc/cowsaya0017f5faf51biohpc_jarekp/cowsay1035e0f20e5fbiohpc/cowsay[jarekp@cbsum1c2b014 ~]\$

COMMAND "/bin/bash" "/bin/bash" "cowsay 'This is Dock"

About a minute ago 9 minutes ago ' 14 minutes ago

CREATED

STATUS o Up About a minute Exited (0) 8 minutes ago Exited (0) 14 minutes ago

PORTS

NAMES jarekp__biohpc_3 jarekp__biohpc_2 jarekp__biohpc_1

The container keeps running in the background! You can execute a command in it, get inside for interactive work, leave it, and it is still there, running.

Run Docker container

• Single command

Run a command and then container stops. docker1 run image command arguments

Interactive mode

Open shell inside container for interactive work. Once you are finished, exit shell and container stops.

docker1 run -it image /bin/bash

Background mode

Start container in the background and connect to it when needed. Container will
keep running.
docker1 run -d -t image /bin/bash
docker1 exec container_id command arguments
docker1 exec -it container_id /bin/bash

Restart container that stopped running (exited)

docker1 start container_id_or_name

docker1 –a –i start container_id_or_name (if restarting in interactive mode)

Docker useful commands summary

- List all conatiners
 docker1 ps -a
- List all images
 docker1 images
- Pull image from a hub docker1 pull image_name
- Load image from <u>save</u> file
 docker1 load -i filename
- Load image from <u>export</u> file docker1 import filename

stop running container
docker1 stop container_id_or_name

remove (erase) container
docker1 rm container_id_or_name

Typically id (e.g. 10af80003f76) or name (e.g. jarekp__biohpc_1) may be used as parameter for stop, rm, exec

BioHPC Docker – cleaning leftovers

Remove all current user non-running containers docker1 clean

Remove all current user containers – running or not docker1 clean all

Automatically remove my container after exit docker1 run --rm image program arguments

By default /workdir/labid is mapped to /workdir inside the container.

You can skip that by using --noworkdir option (in docker1 run command)

Version tag

[jarekp@cbsum1c1b009 ~]\$ docker1 run -it centos:7 /bin/bash Unable to find image 'centos:7' locally Trying to pull repository dtr.cucloud.net/centos ... Trying to pull repository docker.io/library/centos ... sha256:e9ce0b76f29f942502facd92293f1582: Pulling from docker.io/library/centos 524b0c1e57f8: Pull complete Digest: sha256:e9ce0b76f29f942502facd849f3e468232492b259b9d9f076f71b392293f1582 Status: Downloaded newer image for docker.io/centos:7 [root@c0034f8e2cd8 /]# cd /workdir [root@c0034f8e2cd8 workdir]# echo test > myfile [root@c0034f8e2cd8 workdir]# ls -al total 4 File created inside the container is owned by "root" drwxr-xr-x 2 4965 root 20 May 18 19:05 . drwxr-xr-x 1 root root 32 May 18 19:05 ... -rw-r--r-- 1 root root 5 May 18 19:05 myfile [root@c0034f8e2cd8 workdir]# exit



[jarekp@cbsum1c1b009 jarekp]\$ docker1 run --noworkdir -it centos:7 /bin/bash
[root@8f70402109a9 /]# cd /workdir
bash: cd: /workdir: No such file or directory

It is possible to map other directories from host machine to the container inner file system.

The host directory to be mapped must be <u>owned by you</u> and it <u>must be under</u> /workdir/labid/, /local/storage/ or /fs/servername/storage/, /SSD/labid (replace labid with your BioHPC user id)

```
[jarekp@cbsum1c1b009 ~]$ cd /workdir/jarekp/
[jarekp@cbsum1c1b009 jarekp]$ mkdir testdir
[jarekp@cbsum1c1b009 jarekp]$ cd testdir/
[jarekp@cbsum1c1b009 testdir]$ echo test > testfile
```

Mapping /workdir/jarekp/testdir/ outside container to /data inside container Make sure directory name ends with /

```
[jarekp@cbsum1c1b009 testdir]$ docker1 run -v /workdir/jarekp/testdir/:/data -d -t centos:7 /bin/bash
058fb8c312bc415c723dcdaf6842f37c7cb6d3d4dbe092658ac574172da70e69
[jarekp@cbsum1c1b009 testdir]$ docker1 ps -a
CONTAINER ID IMAGE COMMAND CREATED STATUS PORTS NAMES
```

```
058fb8c312bccentos:7"/bin/bash"15 seconds agoUp 13 secondsjarekp__biohpc_4
```

```
[jarekp@cbsum1c1b009 testdir]$ docker1 exec -it 058fb8c312bc /bin/bash
[root@058fb8c312bc /]# cd /data
[root@058fb8c312bc data]# ls -al
total 4
drwxr-xr-x 2 4965 4963 22 May 18 19:15 .
drwxr-xr-x 1 root root 44 May 18 19:15 ..
-rw-r--r-- 1 4965 4963 5 May 18 19:15 testfile
[root@058fb8c312bc data]# cat testfile
test
[root@058fb8c312bc data]#
```

Some Docker images with preinstalled software available from developers require data to be placed in certain directories, often /data. Mapping allows you to satisfy this condition.

You cannot map any directory, only the ones listed above

Docker repositories

Pulled or created Docker images are stored locally on disk in a **local repository/registry**

BioHPC Docker keeps them in /local/docker directory

It is possible to copy local images back to network repositories, provided you have write access to them

Docker repositories

If you modify a container you may want to save it for the future use. Containers and images on rental machines will be deleted once the reservation ends.

You can save container to a file using export command,

or you can convert container to an image and save it to a file with save command, or **push** the image to a hub

In the following example we will start a container using CentOS 7 image, install **htop** program in it and then save it in various ways.

htop is a very useful little program to display server CPU, RAM and I/O usage. It is not a part of default CentOS installation. Sysadmin digression

Many programs and software packages can be installed on Linux with package managers that pull software from software repositories

rpm

They depend on flavor of Linux :

RedHat, CentOSyumDebian, Ubuntuapt-get

All

[jarekp@cbsum1c1b009 ~]\$ docker1 run -d -t centos:7 /bin/bash
829b3f1d48e9e61a462f02714af49d01eac0be34c5f2e41a34ff71f9e68d6b7b
[jarekp@cbsum1c1b009 ~]\$ docker1 ps -a
CONTAINER ID IMAGE COMMAND CREATED STATUS PORTS NAMES
829b3f1d48e9 centos:7 "/bin/bash" 6 seconds ago Up 5 seconds jarekp_biohpc_1
[jarekp@cbsum1c1b009 ~]\$ docker1 exec -it jarekp_biohpc_1 /bin/bash
[root@829b3f1d48e9 /]# htop
bash: htop: command not found

htop is not included in the CentOS 7 system

[root@829b3f1d48e9 /]# yum install htop Loaded plugins: fastestmirror, ovl Determining fastest mirrors * base: mirror.clarkson.edu * extras: mirrors.tripadvisor.com * updates: mirror.siena.edu base extras updates (1/4): base/7/x86 64/group gz (2/4): updates/7/x86 64/primary db (3/4): extras/7/x86_64/primary_db (4/4): base/7/x86_64/primary_db No htop available in these default repositories No package htop available. Error: Nothing to do [root@829b3f1d48e9 /]#

Here is a part of the web page found via Google search "how to install htop on centos 7"

On RHEL/CentOS – 64-bit OS

```
----- For RHEL/CentOS 8 ------
# yum install epel-release [CentOS 8]
# dnf install https://dl.fedoraproject.org/pub/epel/epel-release-latest-8.noarcl
----- For RHEL/CentOS 7 ------
# yum install epel-release
----- For RHEL/CentOS 6 ------
# wget http://download.fedoraproject.org/pub/epel/6/x86 64/epel-release-6-8.noax
# rpm -ihv epel-release-6-8.noarch.rpm
----- For RHEL/CentOS 5 ------
# wget http://download.fedoraproject.org/pub/epel/5/x86_64/epel-release-5-4.noar
# rpm -ihv epel-release-5-4.noarch.rpm
```

[root@829b3f1d48e9 /]# yum install epel-release

Loaded plugins: fastestmirror, ovl

Loading mirror speeds from cached hostfile

* base: mirror.clarkson.edu

* extras: mirrors.tripadvisor.com

* updates: mirror.siena.edu

Resolving Dependencies

--> Running transaction check

---> Package epel-release.noarch 0:7-11 will be installed

--> Finished Dependency Resolution

Dependencies Resolved

[...]

Installed: epel-release.noarch 0:7-11

Complete!
[root@829b3f1d48e9 /]#

```
[root@829b3f1d48e9 /]# yum install htop
Loaded plugins: fastestmirror, ovl
Loading mirror speeds from cached hostfile
epel/x86_64/metalink
```

- * base: mirror.clarkson.edu
- * epel: ftp.cse.buffalo.edu
- * extras: mirrors.tripadvisor.com
- * updates: mirror.siena.edu

[...]

Running transaction
Installing : htop-2.2.0-3.el7.x86_64
Verifying : htop-2.2.0-3.el7.x86_64

Installed:

```
htop.x86_64 0:2.2.0-3.el7
```

Complete!
[root@829b3f1d48e9 /]#

We have now a container with htop. How to save it for later?

```
[jarekp@cbsum1c1b009 ~]$ docker1 ps -a
CONTAINER ID IMAGE COMMAND CREATED STATUS PORTS NAMES
829b3f1d48e9 centos:7 "/bin/bash" 6 seconds ago Up 5 seconds jarekp_biohpc_1
[jarekp@cbsum1c1b009 ~]$ docker1 export -o htop_export.tar jarekp_biohpc_1
```

This command will export the container to a file. The resulting file can be imported to create an image, and then run as a container. What is inside?

```
[jarekp@cbsum1c1b009 ~]$ tar -tf htop_export.tar | more
.dockerenv
anaconda-post.log
bin
dev/
dev/console
dev/pts/
dev/shm/
etc/
etc/.pwd.lock
etc/BUILDTIME
```

Just a list of files – looks like a copy of CentOS system. No special Docker structures.

In order to use save command or push the image to a hub we must create image from the container on hand

container_name image_name
[jarekp@cbsum1c1b009 ~] docker1 commit jarekp__biohpc_1 htop
sha256:515084f37c0ee7995c8b116aaa735ea0dd59b26f7f14daa7ae46b799a5a6ab01

[jarekp@cbsum1c1b009 ~]\$ docker1 images
REPOSITORY TAG IMAGE ID CREATED SIZE
biohpc_jarekp/htop latest 515084f37c0e 56 seconds ago 313 MB
docker.io/centos 7 b5b4d78bc90c 12 days ago 203 MB

htop image is in local private repository **biohpc_jarekp** on the local disk

Now we can save this image to a file

```
[jarekp@cbsum1c1b009 ~]$ cd /workdir/jarekp/
                                              file name
                                                          image name
[jarekp@cbsum1c1b009 jarekp]$ docker1 save -o htop_save.tar biohpc_jarekp/htop
[jarekp@cbsum1c1b009 jarekp]$ ls -al htop_save.tar
-rw----- 1 root root 321216512 May 18 16:26 htop_save.tar
[jarekp@cbsum1c1b009 jarekp]$ tar -tf htop_save.tar | more
tar: htop save.tar: Cannot open: Permission denied
tar: Error is not recoverable: exiting now
[jarekp@cbsum1c1b009 jarekp]$ docker1 claim
[jarekp@cbsum1c1b009 jarekp]$ ls -al htop_save.tar
-rw----- 1 jarekp root 321216512 May 18 16:26 htop_save.tar
[jarekp@cbsum1c1b009 jarekp]$
```

This file is an exact replica of the image, NOT a simple list of files

[jarekp@cbsum1c1b009 jarekp]\$ tar -tf htop_save.tar 0911479852295ffca6aec6236080916bbe7b3e5f1dfda2073d4c9e649346b806/ 0911479852295ffca6aec6236080916bbe7b3e5f1dfda2073d4c9e649346b806/VERSION 0911479852295ffca6aec6236080916bbe7b3e5f1dfda2073d4c9e649346b806/json 0911479852295ffca6aec6236080916bbe7b3e5f1dfda2073d4c9e649346b806/layer.tar 515084f37c0ee7995c8b116aaa735ea0dd59b26f7f14daa7ae46b799a5a6ab01.json f86f06285ab7b035414c42962c83782708058f446cb17b8008791adc4e7832ec/ f86f06285ab7b035414c42962c83782708058f446cb17b8008791adc4e7832ec/VERSION f86f06285ab7b035414c42962c83782708058f446cb17b8008791adc4e7832ec/json f86f06285ab7b035414c42962c83782708058f446cb17b8008791adc4e7832ec/layer.tar manifest.json Repositories

[jarekp@cbsum1c1b009 jarekp]\$

In order to save the image to a hub (registry) we need to

- tag the image with proper name
- login to the hub so it allows us to upload the image
- push the image to the hub

Example below uses our public biohpc repository in docker.io

[jarekp@cbsum1c1b009 jarekp]\$ docker1 tag biohpc_jarekp/htop docker.io/biohpc/htop [jarekp@cbsum1c1b009 jarekp]\$ docker1 images REPOSITORY TAG IMAGE ID CREATED SIZE biohpc_jarekp/htop latest 515084f37c0e 21 minutes ago 313 MB docker.io/biohpc/htop latest 515084f37c0e 21 minutes ago 313 MB

We now have one image (same image ID), but with two names

user registry/hub

[jarekp@cbsum1c1b009 jarekp]\$ docker1 login -u biohpc docker.io Password: Login Succeeded [jarekp@cbsum1c1b009 jarekp]\$ docker1 push docker.io/biohpc/htop The push refers to a repository [docker.io/biohpc/htop] dc3d542d36bd: Pushed edf3aa290fb3: Mounted from library/centos latest: digest: sha256:bb61a8e6e069e74ed26acc9f82eb71663a619a8ec53ad871840c4baa91e6ad4a size: 741 [jarekp@cbsum1c1b009 jarekp]\$ docker1 logout https://index.docker.io/v1/ Removing login credentials for index.docker.io [jarekp@cbsum1c1b009 ~]\$

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