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A Docker container is composed of layers. The layers are combined to create the container. You can think of layers as intermediate images that add some capability to the overall container. If you make a change to a layer through a DockerFile (see Building Containers), than Docker rebuilds that layer and all subsequent layers but not the layers that are not affected by the build. This reduces the time to create containers and also allows you to keep them modular.

Docker is also very good about keeping one copy of the layers on a system. This saves space and also greatly reduces the possibility of "version skew" so that layers that should be the same are not duplicated.

1.1. Hello World For Containers

To make sure you have access to the NVIDIA containers, start with the proverbial “hello world” of Docker commands.

For DGX-2, DGX-1, and DGX Station, simply log into the system. For NGC consult the NGC documentation for details about your specific cloud provider. In general, you will start a cloud instance with your cloud provider using the NVIDIA Volta Deep Learning Image. After the instance has booted, log into the instance.

Next, you can issue the docker --version command to list the version of Docker for DGX-2, DGX-1, and DGX Station. The output of this command tells you the version of Docker on the system (17.05-ce, build 89658be).

At any time, if you are not sure about a Docker command, issue the $ docker --help command.

1.2. Logging Into Docker

If you have a DGX-2, DGX-1, or DGX Station, the first time you login, you are required to set-up access to the NVIDIA NGC Registry (https://ngc.nvidia.com). For more information, see the NGC Getting Started Guide.
1.3. Listing Docker Images

Typically, one of the first things you will want to do is get a list of all the Docker images that are currently available on the local computer. When the Docker containers are stored in a repository, they are said to be a container. When you pull the container from a repository to a system, such as the DGX-2 or DGX-1, it is then said to be a Docker image. This means the image is local.

Issue the $ docker images command to list the images on the server. Your screen will look similar to the following:

![Listing of Docker images](image1)

![Listing of Docker images](image2)

**Figure 1  Listing of Docker images**

and

![Listing of Docker images](image3)

**Figure 2  Listing of Docker images**

In this example, there are a few Docker containers that have been pulled down to this system. Each image is listed along with its tag, the corresponding Image ID, also known as container version. There are two other columns that list when the container was created (approximately), and the approximate size of the image in GB. These columns have been cropped to improve readability.

The output from the command will vary.

At any time, if you need help, issue the $ docker images --help command.
1.4. Pulling A Container

Before you can pull a container from the NGC container registry, you must have Docker and nvidia-docker installed. For DGX users, this is explained in Preparing to use NVIDIA Containers Getting Started Guide.

For users other than DGX, follow the NVIDIA® GPU Cloud™ (NGC) container registry nvidia-docker installation documentation based on your platform.

You must also have access and logged into the NGC container registry as explained in the NGC Getting Started Guide.

Pulling a container to the system makes the container an image. When the container is pulled to become an image, all of the layers are downloaded. Depending upon how many layers are in the container and how the system is connected to the Internet, it may take some time to download.

The $ docker pull nvcr.io/nvidia/tensorflow:17.06 command pulls the container from the NVIDIA repository to the local system where the command is run. At that point, it is a Docker image. The structure of the pull command is:

$ docker pull <repository>/nvidia/<container>:<tag>

Where:

- `<repository>` is the path to where the container is stored (the Docker repo).
  In the following example, the repository is nvcr.io/nvidia (NVIDIA's private repository).
- `<container>` is the name of the container. In the following example we use tensorflow.
- `<xx.xx>` is the specific version of the container. In the following example we use 17.06.

Below is a picture of a TensorFlow image that is pulled using the following command:

$ docker pull nvrc.io/nvidia/tensorflow:17.06
As you can tell, the container had already been pulled down on this particular system (some of the output from the command has been cut off). At this point the image is ready to be run.

In most cases, you will not find a container already downloaded to the system. Below is some sample output for the case when the container has to be pulled down from the registry, using the command:

```bash
$ docker pull nvcr.io/nvidia/tensorflow:17.06
```
Figure 4  Example of pulling TensorFlow 17.06 that had not already been loaded onto the server

Below is the output after the pull is finished, using the command:

$ docker pull nvrc.io/nvidia/tensorflow:17.06
1.5. Running A Container

After the nvidia-docker container is pulled down to the system, creating a Docker image, you can run or execute the image.

**Important** Use the **nvidia-docker** command to ensure that the correct NVIDIA drivers and libraries are used. The next section discusses nvidia-docker.

A typical command to run the container is:

```
nvidia-docker run -it --rm -v local_dir:container_dir nvcr.io/nvidia/<container>:<xx.xx>
```

Where:
- `-it` means interactive
- `--rm` means delete the image when finished
- `-v` means mount directory
local_dir is the directory or file from your host system (absolute path) that you want to access from inside your container. For example, the local_dir in the following path is /home/jsmith/data/mnist.

```bash
-v /home/jsmith/data/mnist:/data/mnist
```

If you are inside the container, for example, `ls /data/mnist`, you will see the same files as if you issued the `ls /home/jsmith/data/mnist` command from outside the container.

container_dir is the target directory when you are inside your container. For example, /data/mnist is the target directory in the example:

```bash
-v /home/jsmith/data/mnist:/data/mnist
```

<container> is the name of the container.

<xx.xx> is the container version, also known as tag. For example, 18.01.

### 1.6. Verifying

After a Docker image is running, you can verify by using the classic *nix option `ps`. For example, issue the `$ docker ps -a` command.

![Figure 6 Verifying a Docker image is running](image)

Without the `-a` option, only running instances are listed.

**Important** It is best to include the `-a` option in case there are hung jobs running or other performance problems.

You can also stop a running container if you want. For example:

![Figure 7 Stopping a container from running](image)

Notice that you need the `Container ID` of the image you want to stop. This can be found using the `$ docker ps -a` command.
Another useful command or Docker option is to remove the image from the server. Removing or deleting the image saves space on the server. For example, issue the following command:

```
$ docker rmi nvcr.io/nvidia.tensorflow:17.06
```

If you list the images, `$ docker images`, on the server, then you will see that the image is no longer there.

```
$ docker images
```

```
REPOSITORY                  TAG       IMAGE ID           CREATED             SIZE
mxnet-dec                   latest    65a48e11da96       19 days ago         127MB
<none>                      <none>    bfc451ca5f2        2 months ago        68MB
nvcr.io/nvidia_general/adlr_pytorch     resumes  a134a99668a8     10 days ago         45MB
<none>                      <none>    04abf6662241       3 months ago        38MB
nvcr.io/nvidia_sas/gamess-libchem     cuda8    97274da5c898     2 months ago        144MB
nvcr.io/nvidia/cuda          latest    6140cdaa05c      2 months ago        230MB
nvcr.io/nvidia/cuda          latest    d355ed3573e9     2 months ago        230MB
```

If you list the images, `$ docker images`, on the server, then you will see that the image is no longer there.

```
$ docker images
```

```
REPOSITORY                  TAG       IMAGE ID           CREATED             SIZE
nvcr.io/nvidia/torch        17.06     b7b62dace81       19 days ago         127MB
nvcr.io/nvidia/cuda         8.0-devel-centos7 7e9e5b71176e 11 days ago         55MB
nvcr.io/nvidia/cuda         8.0-cudnn5-devel-ubuntu14.04 2baf89758249 12 days ago        48MB
nvcr.io/nvidia/cuda         8.0-devel  a76aa0c6fa8 11 days ago         55MB
mxnet/python                <none>    7e9e5b71176e 11 days ago         55MB
nvcr.io/nvidia_sas/chainer  latest    2e70c750b6e 12 days ago         55MB
deep_photo                  latest    ef4510510506 11 days ago         55MB
nvcr.io/nvidia/cuda         <none>    e9243236572f 12 days ago         55MB
nvcr.io/nvidia/tensorflow   17.05     9dd8ed5344f 11 days ago         55MB
bfolks/docker-openvcv       2.4.12-cuda7.0-cudnn4 6f925a3e242b 12 days ago        55MB
```

If you list the images, `$ docker images`, on the server, then you will see that the image is no longer there.
Chapter 2.
DOCKER BEST PRACTICES

You can run an nvidia-docker container on any platform that is Docker compatible allowing you to move your application to wherever you need. The containers are platform-agnostic, and therefore, hardware agnostic as well. To get the best performance and to take full advantage of the tremendous performance of a NVIDIA GPU, specific kernel modules and user-level libraries are needed. NVIDIA GPUs introduce some complexity because they require kernel modules and user-level libraries to operate.

One approach to solving this complexity when using containers is to have the NVIDIA drivers installed in the container and have the character devices mapped corresponding to the NVIDIA GPUs such as /dev/nvidia0. For this to work, the drivers on the host (the system that is running the container), must match the version of the driver installed in the container. This approach drastically reduces the portability of the container.

2.1. nvidia-docker Containers Best Practices

To make things easier for Docker® containers that are built for GPUs, NVIDIA® has created nvidia-docker. It is an open-source project hosted on GitHub. It is basically a wrapper around the docker command that takes care of orchestrating the GPU containers that are needed for your container to run.

Important It is highly recommended you use nvidia-docker when running a Docker container that uses GPUs.

Specifically, it provides two components for portable GPU-based containers.

1. Driver-agnostic CUDA® images
2. A Docker command-line wrapper that mounts the user mode components of the driver and the GPUs (character devices) into the container at launch.
The nvidia-docker containers focus solely on helping you run images that contain GPU dependent applications. Otherwise, it passes the arguments to the regular Docker commands. A good introduction to nvidia-docker is here.

**Important** Some things to always remember:

- Use the `nvidia-docker` command when you are running and executing containers.
- When building containers for NVIDIA GPUs, use the base containers in the repository. This will ensure the containers are compatible with nvidia-docker.

Let's assume the TensorFlow 17.06 container has been pulled down to the system and is now an image that is ready to be run. The following command can be used to execute it.

```bash
$ nvidia-docker run --rm -ti nvcr.io/nvidia/tensorflow:17.06
```

![Figure 11 Executing the `run` command](image)

This takes you to a command prompt inside the container.

**Remember** You are root inside the container.

Running the TensorFlow container didn’t really do anything; it just brought up a command line inside the image where you are root. Below is a better example where the CUDA container is pulled down and the image is executed along with a simple command. This view at least gives you some feedback.
Figure 12  Running an image to give you feedback

This docker image actually executed a command, `nvcc --version`, which provides some output, for example, the version of the nvcc compiler. If you want to get a bash shell in the image then you can run `bash` within the image.

Figure 13  Getting a bash shell in the image

The frameworks that are part of the nvidia-docker repository, `nvcr.io`, have some specific options for achieving the best performance. This is true for DGX-2, DGX-1, and DGX Station. For more information, see Frameworks And Scripts Best Practices.

In the section Using And Mounting File Systems, some options for mounting external file systems in the running image are explained.

Important This allows you to keep data and code stored in one place on the system outside of the containers, while keeping the containers intact.

This also allows the containers to stay generic so they don’t start proliferating when each user creates their own version of the container for their data and code.

2.2. docker exec
There are times when you will need to connect to a running container. You can use the `docker exec` command to connect to a running container to run commands. You can use the `bash` command to start an interactive command line terminal or bash shell.

```
$ docker exec -it <CONTAINER_ID_OR_NAME> bash
```

As an example, suppose one starts a Deep Learning GPU Training System™ (DIGITS) container with the following command:

```
$ nvidia-docker run -d --name test-digits \
- u $(id -u):$(id -g) -e HOME=$HOME -e USER=$USER -v $HOME:$HOME \
  nvcr.io/nvidia/digits:17.05
```

After the container is running, you can now connect to the container instance.

```
$ docker exec -it test-digits bash
```

*test-digits* is the name of the container. If you don’t specifically name the container, you will have to use the container ID.

Important By using `docker exec`, you can execute a snippet of code, a script, or attach interactively to the container making the `docker exec` command very useful.

For detailed usage of the `docker exec` command, see `docker exec`.

### 2.3. `nvcr.io`

Building deep learning frameworks can be quite a bit of work and can be very time consuming. Moreover, these frameworks are being updated weekly, if not daily. On top of this, is the need to optimize and tune the frameworks for GPUs. NVIDIA has created a Docker repository, named `nvcr.io`, where deep learning frameworks are tuned, optimized, tested, and containerized for your use.

NVIDIA creates an updated set of nvidia-docker containers for the frameworks monthly. Included in the container is source (these are open-source frameworks), scripts for building the frameworks, Dockerfiles for creating containers based on these containers, markdown files that contain text about the specific container, and tools and scripts for pulling down datasets that can be used for testing or learning. Customers who purchase a DGX-2, DGX-1 or DGX Station have access to this repository for pushing containers (storing containers).

To get started with DGX-2, DGX-1 or DGX Station, you need to create a system admin account for accessing `nvcr.io`. This account should be treated as an admin account so that users cannot access it. Once this account is created, the system admin can create accounts for projects that belong to the account. They can then give users access to these projects so that they can store or share any containers that they create.

### 2.4. Building Containers
You can build and store containers in the `nvcr.io` registry as a project within your account if you have a DGX-2, DGX-1, or DGX Station (for example, no one else can access the container unless you give them access).

This section of the document applies to Docker containers in general. You can use this general approach for your own Docker repository as well, but be cautious of the details.

Using a DGX-2, DGX-1, or DGX Station, you can either:

1. Create your container from scratch
2. Base your container on an existing Docker container
3. Base your container on containers in `nvcr.io`.

Any one of the three approaches are valid and will work, however, since the goal is to run the containers on a system which has GPUs, it’s logical to assume that the applications will be using GPUs. Moreover, these containers are already tuned for GPUs. All of them also include the needed GPU libraries, configuration files, and tools to rebuild the container.

**Important** Based on these assumptions, it’s recommended that you start with a container from `nvcr.io`.

An existing container in `nvcr.io` should be used as a starting point. As an example, the TensorFlow 17.06 container will be used and Octave will be added to the container so that some post-processing of the results can be accomplished.

1. Pull the container from the NGC container registry to the server. See Pulling A Container.
2. On the server, create a subdirectory called `mydocker`.

   **This is an arbitrary directory name.**

3. Inside this directory, create a file called `Dockerfile` (capitalization is important). This is the default name that Docker looks for when creating a container. The `Dockerfile` should look similar to the following:
Figure 14 Example of a Dockerfile

There are three lines in the **Dockerfile**.

- The first line in the **Dockerfile** tells Docker to start with the container `nvcr.io/nvidia/tensorflow:17.06`. This is the base container for the new container.
- The second line in the **Dockerfile** performs a package update for the container. It doesn’t update any of the applications in the container, but updates the `apt-get` database. This is needed before we install new applications in the container.
- The third and last line in the **Dockerfile** tells Docker to install the package `octave` into the container using `apt-get`.

The Docker command to create the container is:

```
$ docker build -t nvcr.io/nvidia_sas/tensorflow_octave:17.06_with_octave
```

```
RUN apt-get update
RUN apt-get install -y octave
```

This command uses the default file **Dockerfile** for creating the container.

The command starts with `docker build`. The `-t` option creates a tag for this new container. Notice that the tag specifies the project in the `nvcr.io` repository where the container is to be stored. As an example, the project `nvidia_sas` was used along with the repository `nvcr.io`.

Projects can be created by your local administrator who controls access to `nvcr.io`, or they can give you permission to create them. This is where you can store your specific containers and even share them with your colleagues.
Figure 15  Creating a container using the Dockerfile

In the brief output from the `docker build` ... command shown above, each line in the Dockerfile is a Step. In the screen capture, you can see the first and second steps (commands). Docker echos these commands to the standard out (`stdout`) so you can watch what it is doing or you can capture the output for documentation.

After the image is built, remember that we haven't stored the image in a repository yet, therefore, it's a Docker image. Docker prints out the image id to `stdout` at the very end. It also tells you if you have successfully created and tagged the image.

If you don’t see Successfully ... at the end of the output, examine your Dockerfile for errors (perhaps try to simplify it) or try a very simple Dockerfile to ensure that Docker is working properly.

4. Verify that Docker successfully created the image.

```
$ docker images
```

Figure 16  Verifying Docker created the image
The very first entry is the new image (about 1 minute old).

5. Push the image into the repository, creating a container.

```
docker push <name of image>
```

![Example of the `docker push` command](image)

**Figure 17  Example of the docker push command**

The above screen capture is after the `docker push` command pushes the image to the repository creating a container. At this point, you should log into the NGC container registry at [https://ngc.nvidia.com](https://ngc.nvidia.com) and look under your project to see if the container is there.

If you don’t see the container in your project, make sure that the tag on the image matches the location in the repository. If, for some reason, the push fails, try it again in case there was a communication issue between your system and the container registry ([nvcr.io](https://nvcr.io)).

To make sure that the container is in the repository, we can pull it to the server and run it. As a test, first remove the image from your DGX system using the command `docker rmi` .... Then, pull the container down to the server using `docker pull` .... The image can be run using `nvidia-docker` as shown below.
Figure 18  Example of using `nvidia-docker` to pull container

Notice that the `octave` prompt came up so it is installed and functioning correctly within the limits of this testing.

2.5. Using And Mounting File Systems

One of the fundamental aspects of using Docker is mounting file systems inside the Docker container. These file systems can contain input data for the frameworks or even code to run in the container.

Docker containers have their own internal file system that is separate from file systems on the rest of the host.

**Important** You can copy data into the container file system from outside if you want. However, it’s far easier to mount an outside file system into the container.

Mounting outside file systems is done using the `nvidia-docker` command and the `-v` option. For example, the following command mounts two file systems:

```bash
$ nvidia-docker run --rm -ti ... -v $HOME:$HOME \
   -v /datasets/digits_data:ro \
   ...
```

Most of the command has been erased except for the volumes. This command mounts the user’s home directory from the external file system to the home directory in the
container (-v $HOME:$HOME). It also takes the /datasets directory from the host and mounts it on /digits_data inside the container (-v /datasets:/digits_data:ro).

Remember: The user has root privileges with Docker, therefore you can mount almost anything from the host system to anywhere in the container.

For this particular command, the volume command takes the form of:

```
-v <External FS Path>:<Container FS Path>(options) \
```

The first part of the option is the path for the external file system. To be sure this works correctly, it’s best to use the fully qualified path (FQP). This is also true for the mount point inside the container <Container FS Path>.

After the last path, various options can be used in the parenthesis (). In the above example, the second file system is mounted read-only (ro) inside the container. The various options for the -v option are discussed here.

The DGX™ systems (DGX-2, DGX-1, and DGX Station), and the nvidia-docker containers use the Overlay2 storage driver to mount external file systems onto the container file system. Overlay2 is a union-mount file system driver that allows you to combine multiple file systems so that all the content appears to be combined into a single file system. It creates a union of the file systems rather than an intersection.
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