https://researchcomputing.princeton.edu/singularity
FROM ubuntu:20.04
USER root
RUN apt-get -y update \
&& DEBIAN_FRONTEND=noninteractive apt-get install -y --no-install-recommends build-essential cmake wget
RUN mkdir -p /opt/data && mkdir /mytemp && cd /mytemp \
&& mkdir build && cd build
RUN cmake -D CMAKE_INSTALL_PREFIX=/opt \
   -D BUILD_MPI=no -D BUILD_OMP=no -D CMAKE_BUILD_TYPE=Release \
   -D CMAKE_CXX_FLAGS_RELEASE=-O3 -D PKG_MOLECULE=yes /mytemp/lammps-stable_29Oct2020/cmake
RUN make -j 4 && make install && rm -rf /mytemp
ENV PATH="/opt/bin:$PATH"
COPY in.melt /opt/data
ENTRYPOINT ["lmp", "-in", "/opt/data/in.melt"]
#USER jhalverson

$ docker build --tag jhalverson/lammps:image1 --file Dockerfile .
$ docker run -it --rm jhalverson/lammps:image1
$ docker push jhalverson/lammps:image1
How to deal with large Singularity files

Adroit

```bash
export SINGULARITY_CACHEDIR=/scratch/network/$USER/SINGULARITY_CACHE
export SINGULARITY_TMPDIR=/tmp
```

Della, Stellar, Tiger, Traverse

```bash
export SINGULARITY_CACHEDIR=/scratch/gpfs/$USER/SINGULARITY_CACHE
export SINGULARITY_TMPDIR=/tmp
```
Hands-on Exercise 1

1. Browse to Docker Hub and find a "lolcow" container by sylabsio (i.e., search "lolcow sylabsio")

2. The search should take you to this webpage: https://hub.docker.com/r/sylabsio/lolcow

3. Pull the image to Adroit and run it (Hint: you need to convert docker pull sylabsio/lolcow:latest)
Hands-on Exercise 1

1. Browse to Docker Hub and find a "lolcow" container by sylabsio (i.e., search "lolcow sylabsio")

2. The search should take you to this webpage: https://hub.docker.com/r/sylabsio/lolcow

3. Pull the image to Adroit and run it (Hint: you need to convert docker pull sylabsio/lolcow:latest)

Solution

$ ssh <YourNetID>@adroit.princeton.edu
$ singularity pull docker://sylabsio/lolcow:latest
$ singularity run lolcow_latest.sif
$ ./lolcow_latest.sif
$ singularity exec lolcow_latest.sif cowsay "Containers are cool"
$ singularity exec lolcow_latest.sif cowsay "Containers are cool" | singularity exec lolcow_latest.sif lolcat
Hands-on Exercise 2

Find the "jhalverson" "lammps" image on Docker Hub. Pull it on Adroit and run it.
Hands-on Exercise 2

Find the "jhalverson" "lammps" image on Docker Hub. Pull it on Adroit and run it.

Solution

$ ssh <YourNetID>@adroit.princeton.edu
$ singularity pull docker://jhalverson/lammps:image1
$ singularity run lammps_image1.sif
Hands-on Exercise 3

"Shell into" the container to explore it:

$ singularity shell lolcow_latest.sif
Singularity> whoami
...
Singularity> hostname
...
Singularity> cat /etc/os-release
...
Singularity> exit
...
$ cat /etc/os-release
...
Hands-on Exercise 4

Create a bind mount to /home/jdh4/software. There is a file in that directory called message.txt. Run cowsay on that file (i.e., cowsay < /name-of-bind-mount/message.txt).
Hands-on Exercise 4

Create a bind mount to /home/jdh4/software. There is a file in that directory called message.txt. Run cowsay on that file (i.e., cowsay < /name-of-bind-mount/message.txt).

Solution

$ singularity shell -B /home/jdh4/software:/mymount lolcow_latest.sif
Singularity> cd /mymount
Singularity> ls -l
...
Singularity> cowsay < message.txt
...
Singularity> exit

use redirection to send the contents of message.txt to cowsay
Hands-on Exercise 5

Find the location of the file in.melt in lammps_image1.sif. Use "singularity shell" and "--containall" so that only the container is searched when using the find command.
Hands-on Exercise 5

Find the location of the file `in.melt` in `lammps_image1.sif`. Use "singularity shell" and "--containall" so that only the container is searched when using the `find` command.

Solution

```bash
$ singularity pull docker://jhalverson/lammps:image1
$ singularity shell --containall lammps_image1.sif
Singularity> find / -iname "*in.melt*" 2>/dev/null
...  
Singularity> exit
```

`ignore error messages`