

<https://researchcomputing.princeton.edu/singularity>

Dockerfile

```
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 \
  && wget --no-check-certificate https://github.com/lammps/lammps/archive/stable_29oct2020.tar.gz \
  && tar xzf stable_29oct2020.tar.gz && cd lammps-stable_29oct2020 \
  && 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

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

Della, Stellar, Tiger, Traverse

```
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`)

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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" "lammmps" image on Docker Hub. Pull it on Adroit and run it.

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

Solution

```
$ ssh <YourNetID>@adroit.princeton.edu  
$ singularity pull docker://jhalverson/lammers:image1  
$ singularity run lammers_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

```
$ 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*