ALCF COMPUTATIONAL PERFORMANCE WORKSHOP

MAY 4-6, 2021

CONTAINERS ON THETA AND THETA-GPU AN INTRODUCTION

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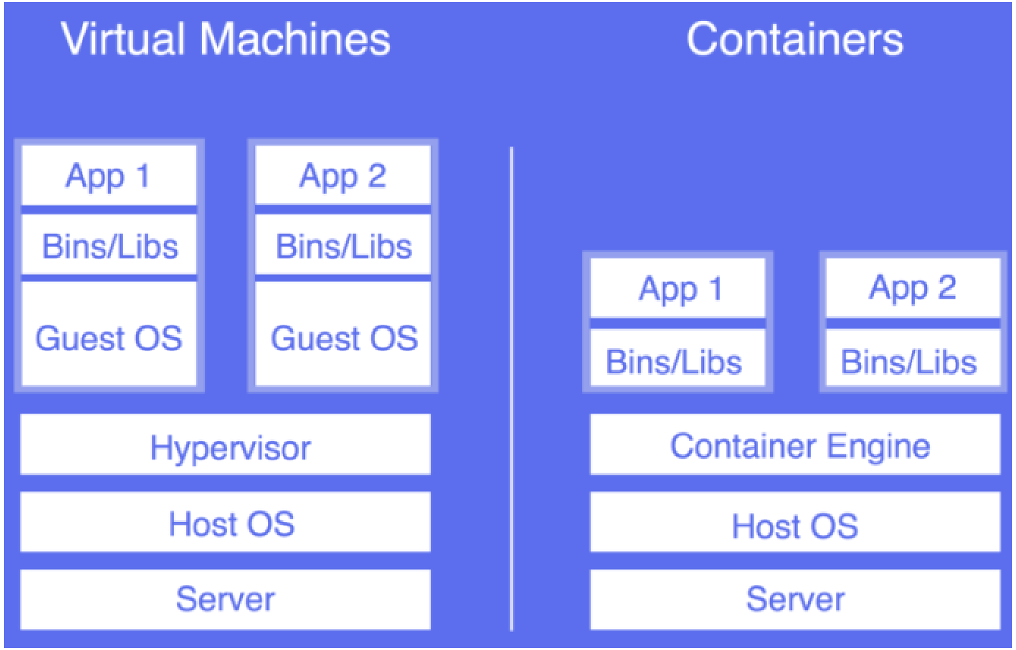
Outline

- Using singularity containers on Theta and Theta-GPU
- Using Docker-hub to build containers and build them using Singularity on Theta (for running MPI apps).
- Using pre-existing singularity images on Theta-GPU for deep learning workloads.
- When in doubt – message us on the CPW portal.

Containers

- Lightweight alternatives to virtual machines and increasingly popular for cloud applications. Examples: Docker, Singularity, Rocket etc.



Singularity is our container of choice for security reasons.

However, Docker is the most widely used container platform.

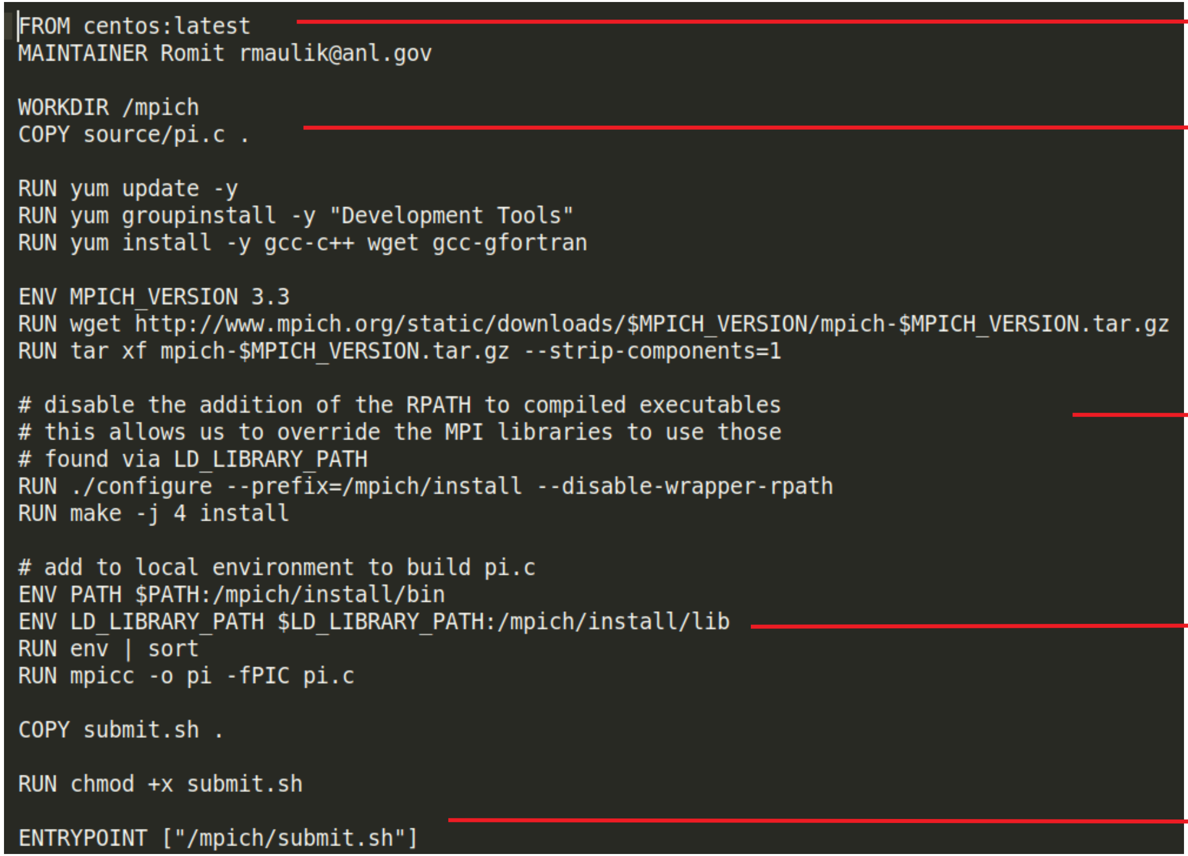
Dockerfiles and Docker-hub

- Option 1: Build a docker image on their local machine and upload to docker-hub (needs local installation of docker).
- Option 2: Link Github and docker-hub and auto-build using Dockerfile. (does not need local installation but useful for testing anyway).
- We'll show you how docker and docker-hub can be used to port your docker containers to Theta and build Singularity images.
- Due to time constraints – we cannot show you how to install docker on your local machine (but this is not very difficult):

  Visit: https://docs.docker.com/engine/install/ and choose your OS.

  Our results/demos today from docker version 20.10.6

An example Dockerfile



```
FROM centos:latest
MAINTAINER Romit rmaulik@anl.gov

WORKDIR /mpich
COPY source/pi.c .

RUN yum update -y
RUN yum groupinstall -y "Development Tools"
RUN yum install -y gcc-c++ wget gcc-gfortran

ENV MPICH_VERSION 3.3
RUN wget http://www.mpich.org/static/downloads/$MPICH_VERSION/mpich-$MPICH_VERSION.tar.gz
RUN tar xf mpich-$MPICH_VERSION.tar.gz --strip-components=1

# disable the addition of the RPATH to compiled executables
# this allows us to override the MPI libraries to use those
# found via LD_LIBRARY_PATH
RUN ./configure --prefix=/mpich/install --disable-wrapper-rpath
RUN make -j 4 install

# add to local environment to build pi.c
ENV PATH $PATH:/mpich/install/bin
ENV LD_LIBRARY_PATH $LD_LIBRARY_PATH:/mpich/install/lib
RUN env | sort
RUN mpicc -o pi -fPIC pi.c

COPY submit.sh .

RUN chmod +x submit.sh

ENTRYPOINT ["/mpich/submit.sh"]
```

Container OS pulled from docker-hub repository

Working directory in container – copy source

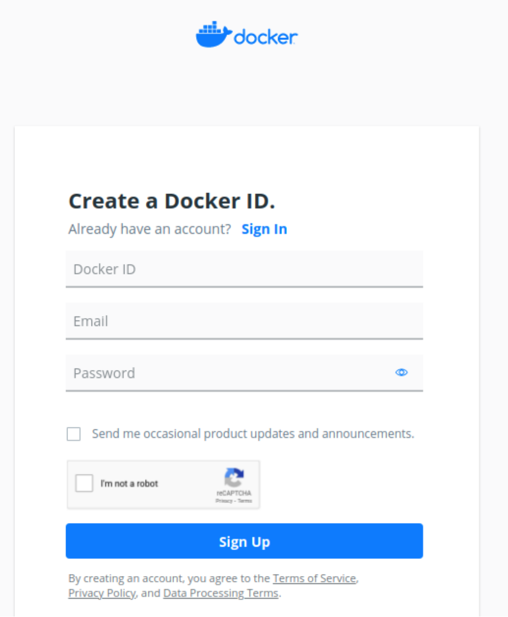
Install appropriate packages for building app

Build your app

Specify script to run and copy from local

Linking Github and Docker-hub

- Make sure you have both Github and Docker-hub accounts (sign up with email).



docker

Create a Docker ID.

Already have an account? Sign In

Docker ID

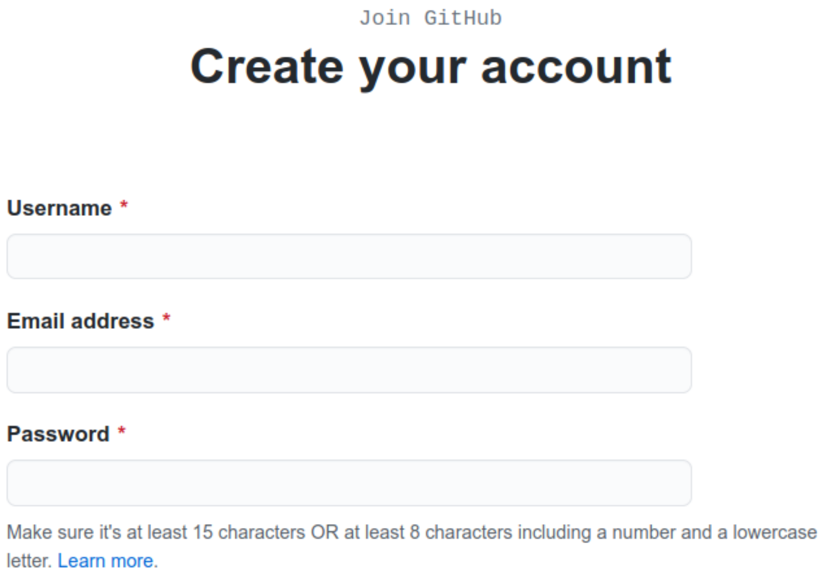
Email

Password

□ Send me occasional product updates and announcements.

□ I'm not a robot

By creating an account, you agree to the Terms of Service, Privacy Policy, and Data Processing Terms.



Join GitHub

Create your account

Username *

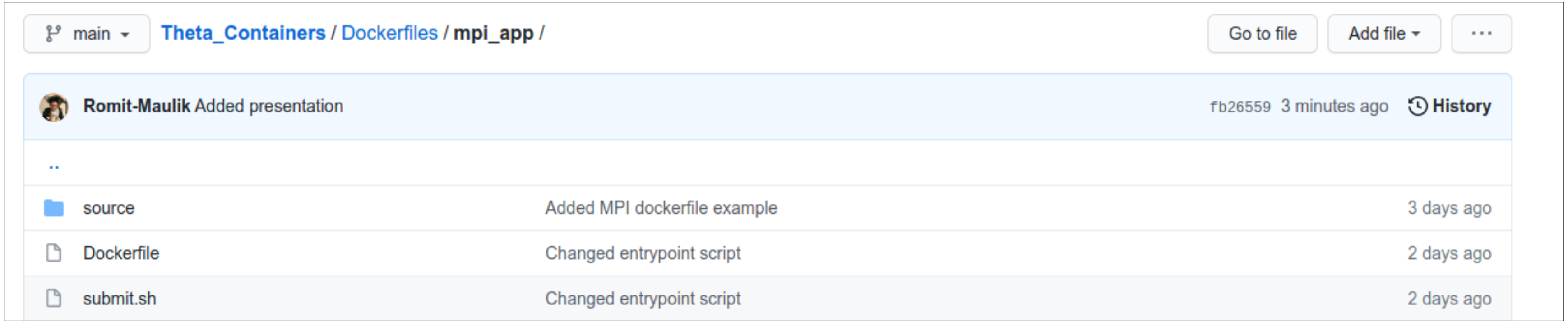
Email address *

Password *

Make sure it's at least 15 characters OR at least 8 characters including a number and a lowercase letter. Learn more.

Linking Github and Docker-hub

- Make sure you have both Github and Docker-hub accounts (sign up with email).
- Push your Dockerfile to a github repository



Theta_Containers / Dockerfiles / mpi_app /

Romit-Maulik Added presentation fb26559 3 minutes ago

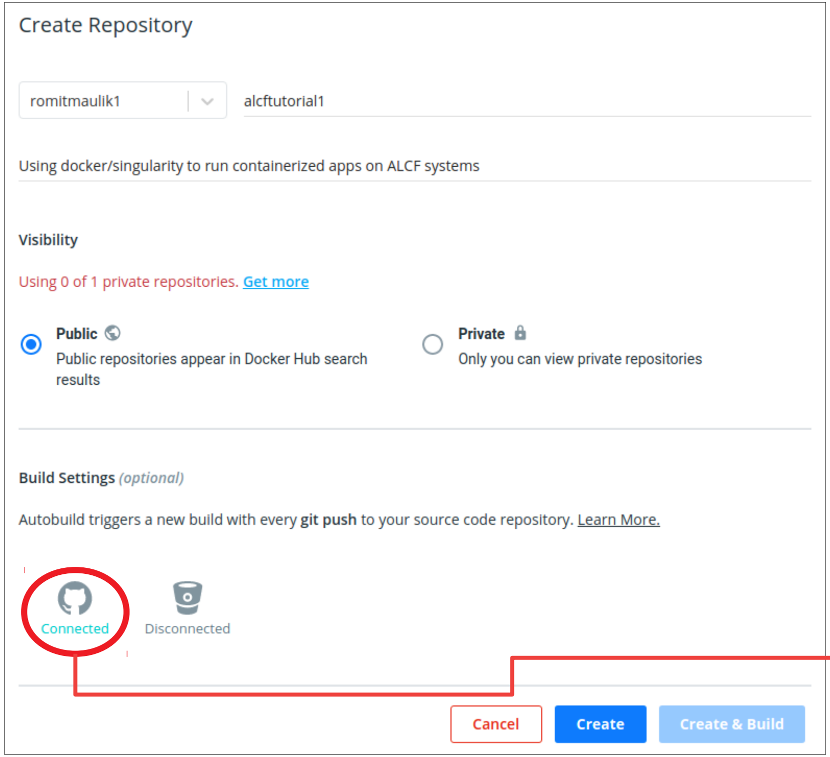
..

source	Added MPI dockerfile example	3 days ago
Dockerfile	Changed entrypoint script	2 days ago
submit.sh	Changed entrypoint script	2 days ago

Example code at
https://github.com/Romit-Maulik/Theta_Containers/

Linking Github and Docker-hub

- Link that repository with a Docker-hub repository



Create Repository

romitmaulik1 | alcftutorial1

Using docker/singularity to run containerized apps on ALCF systems

Visibility

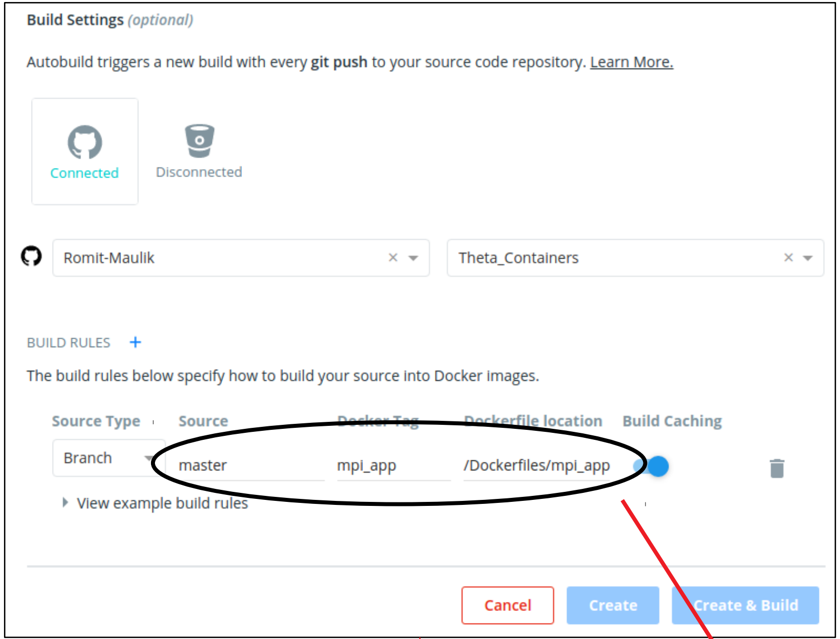
Using 0 of 1 private repositories. Get more

● **Public** Public repositories appear in Docker Hub search results

○ **Private** Only you can view private repositories

Build Settings *(optional)*

Autobuild triggers a new build with every **git push** to your source code repository. Learn More.



Build Settings *(optional)*

Autobuild triggers a new build with every **git push** to your source code repository. Learn More.

Romit-Maulik | Theta_Containers

BUILD RULES +

The build rules below specify how to build your source into Docker images.

Source Type	Source	Docker Tag	Dockerfile location	Build Caching
Branch	master	mpi_app	/Dockerfiles/mpi_app	●

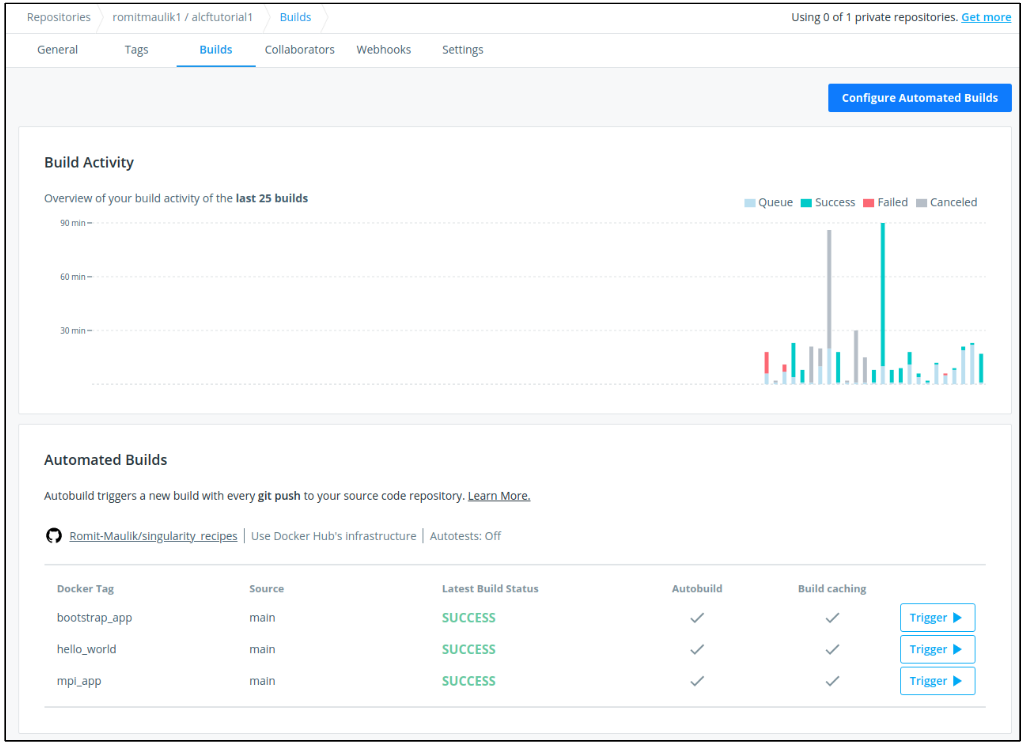
▸ View example build rules

This will be disconnected the first time

Specify branch, image name (tag), path to docker file in repo

Linking Github and Docker-hub

- Building on docker-hub is slow (when compared to your local machine) but once complete you should see something like this



Repositories › romitmaulik1 / alcftutorial1 › Builds

Using 0 of 1 private repositories. Get more

Build Activity

Overview of your build activity of the **last 25 builds**

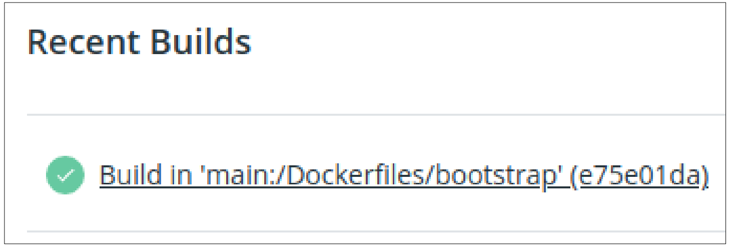
Automated Builds

Autobuild triggers a new build with every **git push** to your source code repository. Learn More.

Romit-Maulik/singularity_recipes | Use Docker Hub's infrastructure | Autotests: Off

Docker Tag	Source	Latest Build Status	Autobuild	Build caching	
bootstrap_app	main	SUCCESS	✓	✓	Trigger ▶
hello_world	main	SUCCESS	✓	✓	Trigger ▶
mpi_app	main	SUCCESS	✓	✓	Trigger ▶

Using “Configure Automated Builds” to edit build names (tags), paths etc.



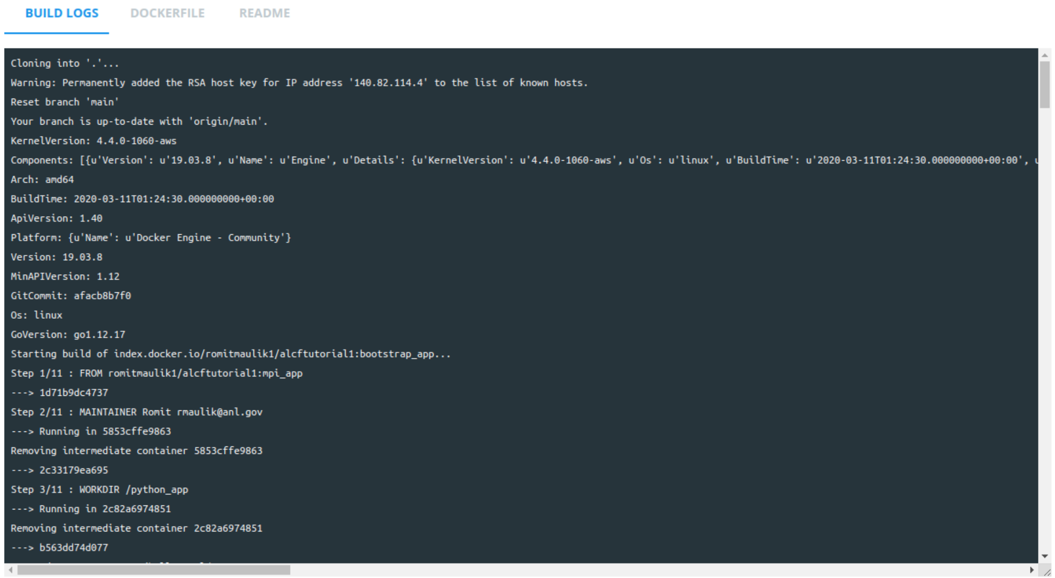
Recent Builds

✓ Build in 'main:/Dockerfiles/bootstrap' (e75e01da)

Clicking on a recent build with give you logs (useful for debugging fails) and the docker file itself.

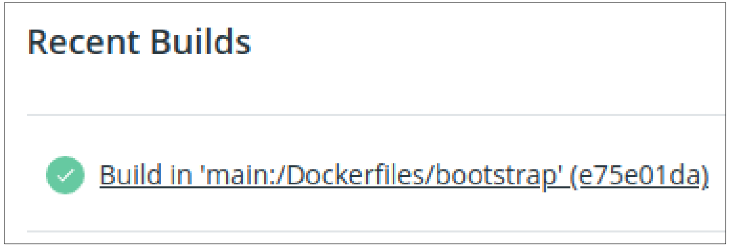
Linking Github and Docker-hub

- Building on docker-hub is slow (when compared to your local machine) but once complete you should see something like this



```
Cloning into '.'...
Warning: Permanently added the RSA host key for IP address '140.82.114.4' to the list of known hosts.
Reset branch 'main'
Your branch is up-to-date with 'origin/main'.
KernelVersion: 4.4.0-1060-aws
Components: [{u'Version': u'19.03.8', u'Name': u'Engine', u'Details': {u'KernelVersion': u'4.4.0-1060-aws', u'Os': u'linux', u'BuildTime': u'2020-03-11T01:24:30.000000000+00:00', u
Arch: amd64
BuildTime: 2020-03-11T01:24:30.000000000+00:00
ApiVersion: 1.40
Platform: {u'Name': u'Docker Engine - Community'}
Version: 19.03.8
MinAPIVersion: 1.12
GitCommit: afacb8b7f0
Os: linux
GoVersion: go1.12.17
Starting build of index.docker.io/romitmaulik1/alcftutorial1:bootstrap_app...
Step 1/11 : FROM romitmaulik1/alcftutorial1:mpi_app
---> 1d71b9dc4737
Step 2/11 : MAINTAINER Romit rmaulik@anl.gov
---> Running in 5853cffe9863
Removing intermediate container 5853cffe9863
---> 2c33179ea695
Step 3/11 : WORKDIR /python_app
---> Running in 2c82a6974851
Removing intermediate container 2c82a6974851
---> b563dd74d077
```

Using “Configure Automated Builds” to edit build names (tags), paths etc.



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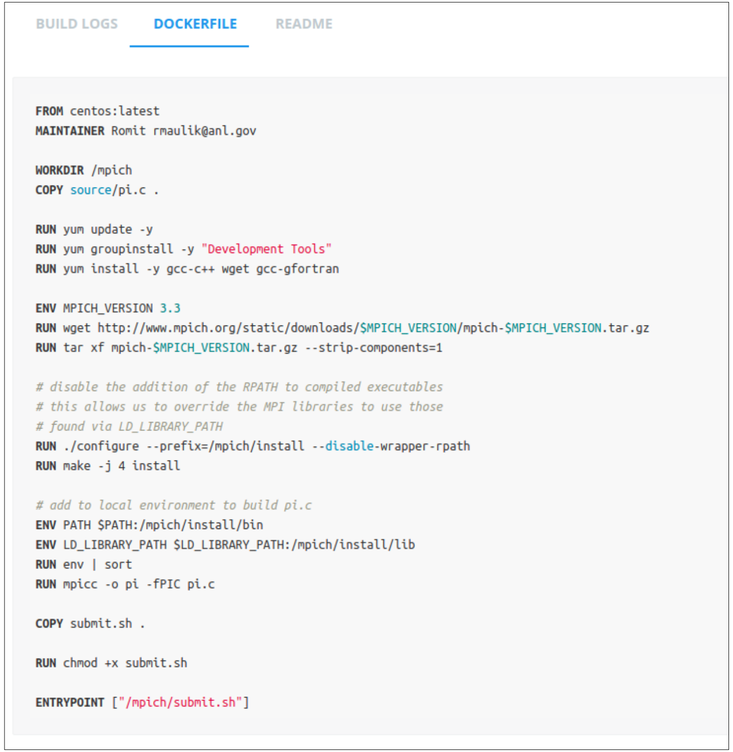

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ENV LD_LIBRARY_PATH $LD_LIBRARY_PATH:/mpich/install/lib
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RUN mpicc -o pi -fPIC pi.c

COPY submit.sh .

RUN chmod +x submit.sh

ENTRYPOINT ["/mpich/submit.sh"]
```

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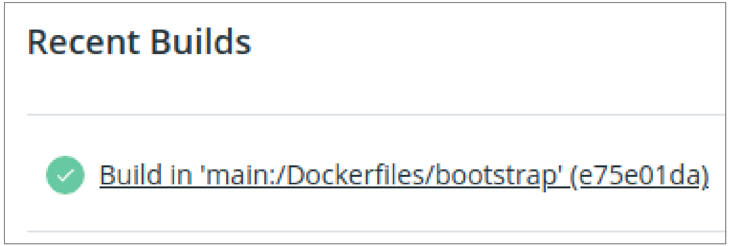


Clicking on a recent build with give you logs (useful for debugging fails) and the docker file itself.

Pulling image to Theta

- Once build is successful on Docker-hub – pull to Theta using singularity (version 3.6.4-1)
- Command:

singularity build mpi_app.img docker://romitmaulik1/alcftutorial1:mpi_app

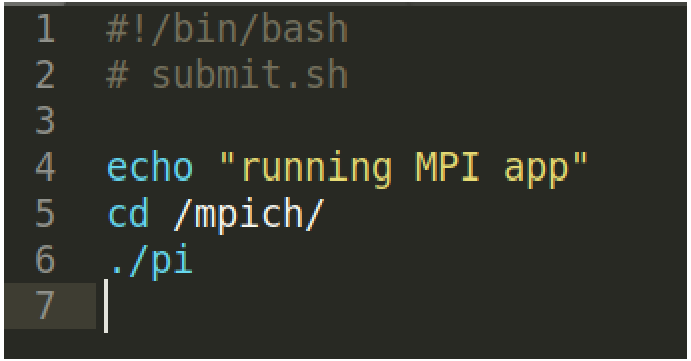
- Explore the contents of your image with:

singularity shell mpi_app.img

- You can find your source code, downloaded libraries, submit scripts in

ls /mpich/

- Your entrypoint script will look like



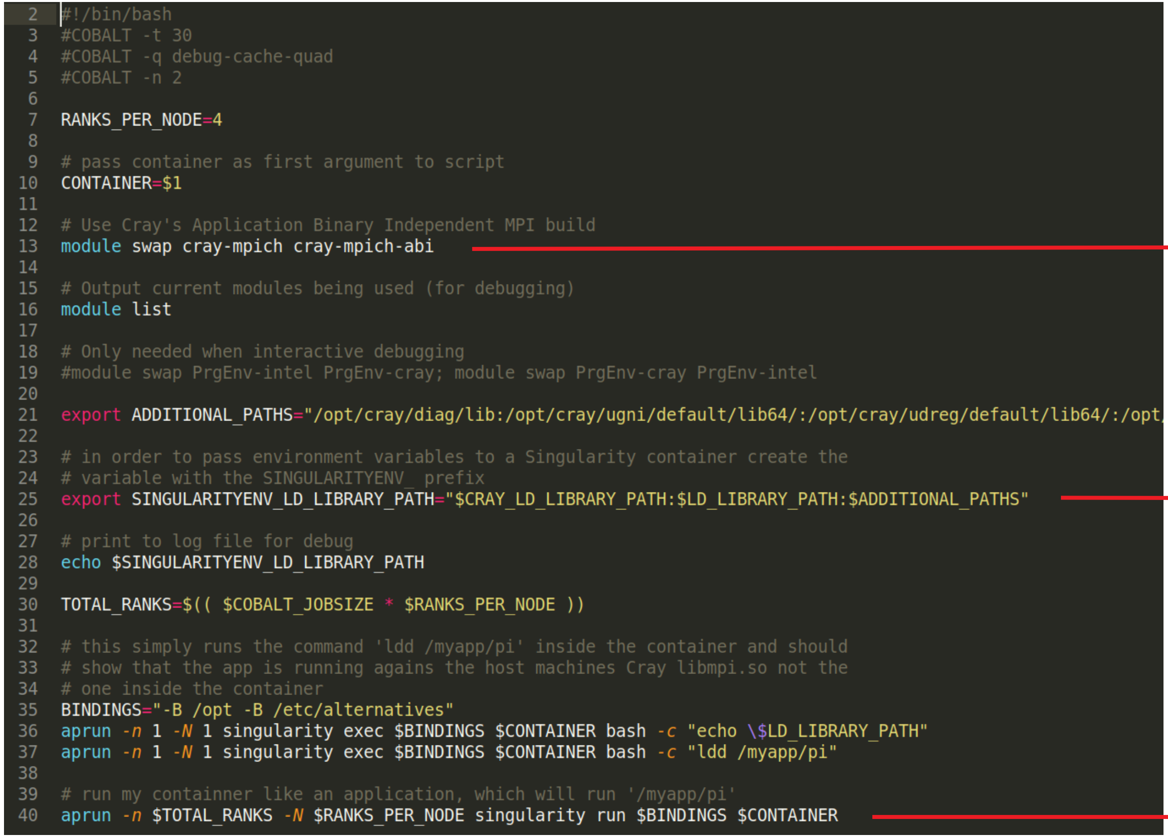
```
#!/bin/bash
# submit.sh

echo "running MPI app"
cd /mpich/
./pi

```

Interface MPI apps with Theta

- We need to swap out binaries with Cray in the submission script



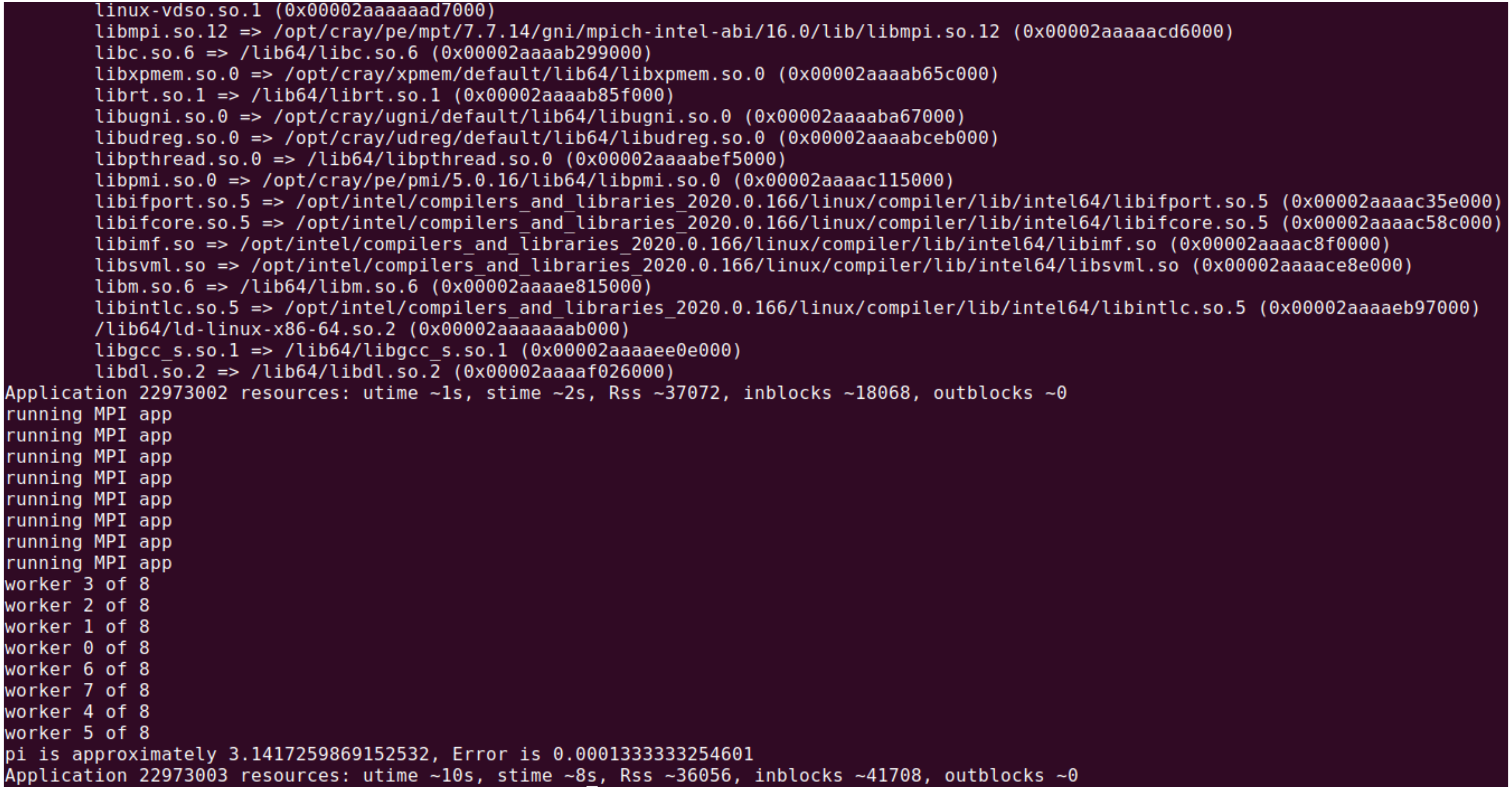
```bash
#!/bin/bash
#COBALT -t 30
#COBALT -q debug-cache-quad
#COBALT -n 2

RANKS_PER_NODE=4

# pass container as first argument to script
CONTAINER=$1

# Use Cray's Application Binary Independent MPI build
module swap cray-mpich cray-mpich-abi

# Output current modules being used (for debugging)
module list

# Only needed when interactive debugging
#module swap PrgEnv-intel PrgEnv-cray; module swap PrgEnv-cray PrgEnv-intel

export ADDITIONAL_PATHS="/opt/cray/diag/lib:/opt/cray/ugni/default/lib64/:/opt/cray/udreg/default/lib64/:/opt/

# in order to pass environment variables to a Singularity container create the
# variable with the SINGULARITYENV_ prefix
export SINGULARITYENV_LD_LIBRARY_PATH="$CRAY_LD_LIBRARY_PATH:$LD_LIBRARY_PATH:$ADDITIONAL_PATHS"

# print to log file for debug
echo $SINGULARITYENV_LD_LIBRARY_PATH

TOTAL_RANKS=$(( $COBALT_JOBSIZE * $RANKS_PER_NODE ))

# this simply runs the command 'ldd /myapp/pi' inside the container and should
# show that the app is running agains the host machines Cray libmpi.so not the
# one inside the container
BINDINGS="-B /opt -B /etc/alternatives"
aprun -n 1 -N 1 singularity exec $BINDINGS $CONTAINER bash -c "echo \$LD_LIBRARY_PATH"
aprun -n 1 -N 1 singularity exec $BINDINGS $CONTAINER bash -c "ldd /myapp/pi"

# run my containner like an application, which will run '/myapp/pi'
aprun -n $TOTAL_RANKS -N $RANKS_PER_NODE singularity run $BINDINGS $CONTAINER
```

Use cray-mpich-abi for compatibility with your build (remember to check compatibility of versions of mpich and cray-mpich)

Pass paths to CRAY objects to your container using SINGULARITYENV_LD_LIBRARY_PATH

Run using aprun

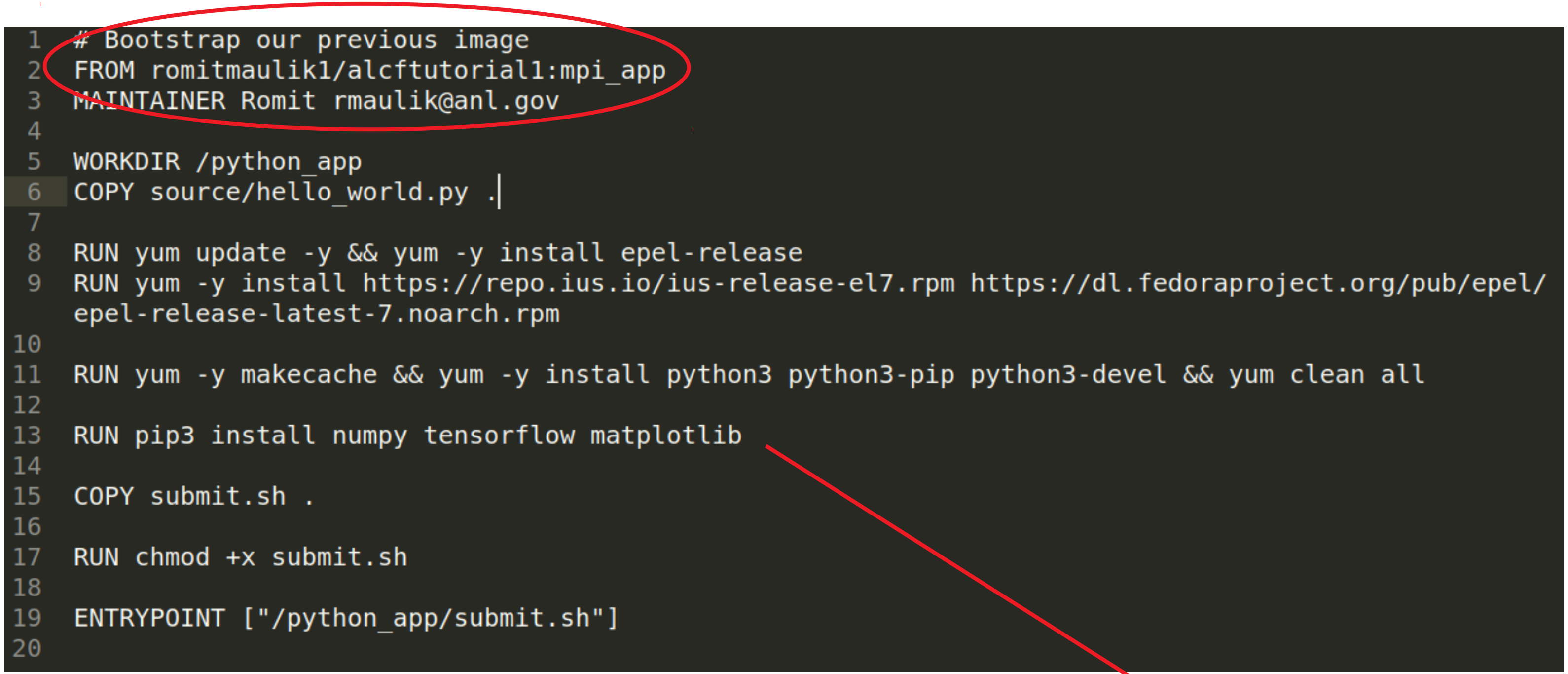
What is finally observed



```
        linux-vdso.so.1 (0x00002aaaaaad7000)
        libmpi.so.12 => /opt/cray/pe/mpt/7.7.14/gni/mpich-intel-abi/16.0/lib/libmpi.so.12 (0x00002aaaaacd6000)
        libc.so.6 => /lib64/libc.so.6 (0x00002aaaab299000)
        libxpmem.so.0 => /opt/cray/xpmem/default/lib64/libxpmem.so.0 (0x00002aaaab65c000)
        librt.so.1 => /lib64/librt.so.1 (0x00002aaaab85f000)
        libugni.so.0 => /opt/cray/ugni/default/lib64/libugni.so.0 (0x00002aaaaba67000)
        libudreg.so.0 => /opt/cray/udreg/default/lib64/libudreg.so.0 (0x00002aaaabceb000)
        libpthread.so.0 => /lib64/libpthread.so.0 (0x00002aaaabef5000)
        libpmi.so.0 => /opt/cray/pe/pmi/5.0.16/lib64/libpmi.so.0 (0x00002aaaac115000)
        libifport.so.5 => /opt/intel/compilers_and_libraries_2020.0.166/linux/compiler/lib/intel64/libifport.so.5 (0x00002aaaac35e000)
        libifcore.so.5 => /opt/intel/compilers_and_libraries_2020.0.166/linux/compiler/lib/intel64/libifcore.so.5 (0x00002aaaac58c000)
        libimf.so => /opt/intel/compilers_and_libraries_2020.0.166/linux/compiler/lib/intel64/libimf.so (0x00002aaaac8f0000)
        libsvml.so => /opt/intel/compilers_and_libraries_2020.0.166/linux/compiler/lib/intel64/libsvml.so (0x00002aaaace8e000)
        libm.so.6 => /lib64/libm.so.6 (0x00002aaaae815000)
        libintlc.so.5 => /opt/intel/compilers_and_libraries_2020.0.166/linux/compiler/lib/intel64/libintlc.so.5 (0x00002aaaaeb97000)
        /lib64/ld-linux-x86-64.so.2 (0x00002aaaaaaab000)
        libgcc_s.so.1 => /lib64/libgcc_s.so.1 (0x00002aaaaee0e000)
        libdl.so.2 => /lib64/libdl.so.2 (0x00002aaaaf026000)
Application 22973002 resources: utime ~1s, stime ~2s, Rss ~37072, inblocks ~18068, outblocks ~0
running MPI app
running MPI app
running MPI app
running MPI app
running MPI app
running MPI app
running MPI app
running MPI app
worker 3 of 8
worker 2 of 8
worker 1 of 8
worker 0 of 8
worker 6 of 8
worker 7 of 8
worker 4 of 8
worker 5 of 8
pi is approximately 3.1417259869152532, Error is 0.0001333333254601
Application 22973003 resources: utime ~10s, stime ~8s, Rss ~36056, inblocks ~41708, outblocks ~0
```

Bootstrapping

- When possible reuse previous builds in opensource repositories



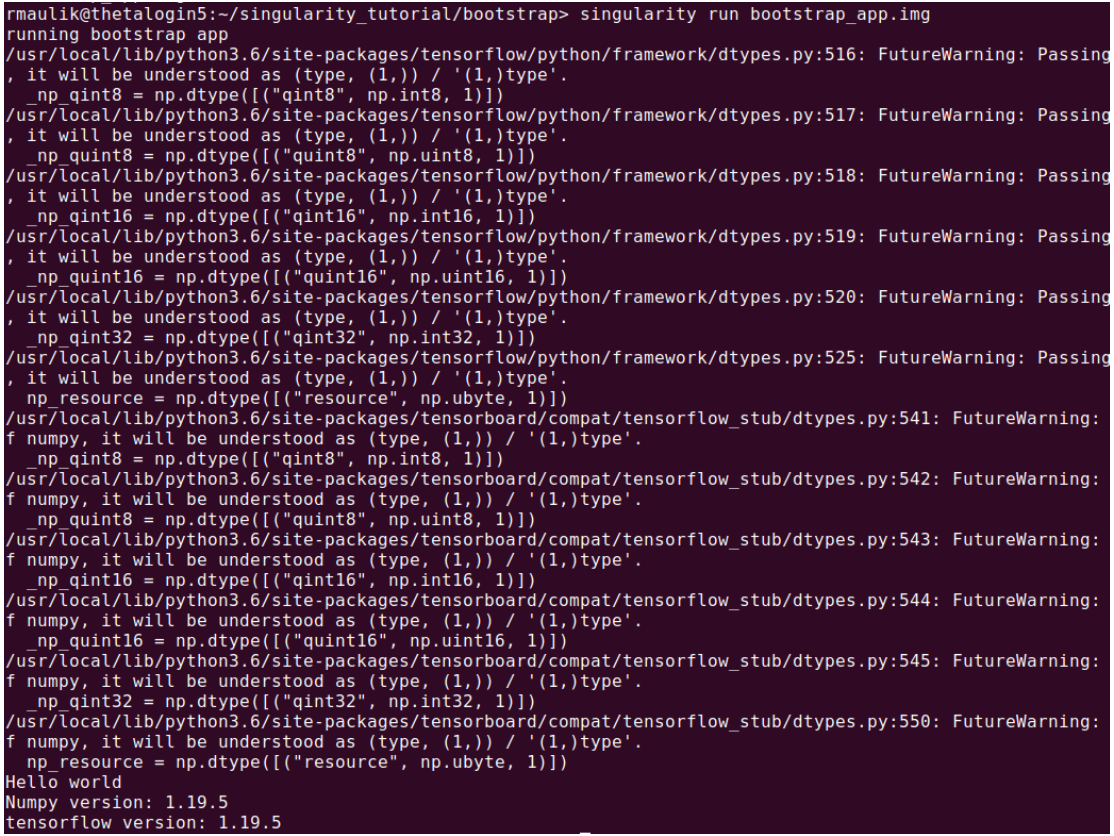
```
# Bootstrap our previous image
FROM romitmaulik1/alcftutorial1:mpi_app
MAINTAINER Romit rmaulik@anl.gov

WORKDIR /python_app
COPY source/hello_world.py .

RUN yum update -y && yum -y install epel-release
RUN yum -y install https://repo.ius.io/ius-release-el7.rpm https://dl.fedoraproject.org/pub/epel/epel-release-latest-7.noarch.rpm

RUN yum -y makecache && yum -y install python3 python3-pip python3-devel && yum clean all

RUN pip3 install numpy tensorflow matplotlib

COPY submit.sh .

RUN chmod +x submit.sh

ENTRYPOINT ["/python_app/submit.sh"]

```

We add a python application into this pre-existing image and build a new one

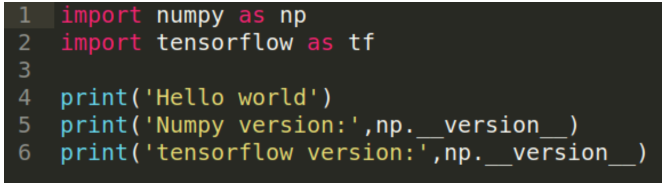
Install some common datascience packages

Bootstrapping

- When possible reuse previous builds in opensource repositories



```
rmaulik@thetalogin5:~/singularity_tutorial/bootstrap> singularity run bootstrap_app.img
running bootstrap app
/usr/local/lib/python3.6/site-packages/tensorflow/python/framework/dtypes.py:516: FutureWarning: Passing
, it will be understood as (type, (1,)) / '(1,)type'.
  _np_qint8 = np.dtype([("qint8", np.int8, 1)])
/usr/local/lib/python3.6/site-packages/tensorflow/python/framework/dtypes.py:517: FutureWarning: Passing
, it will be understood as (type, (1,)) / '(1,)type'.
  _np_quint8 = np.dtype([("quint8", np.uint8, 1)])
/usr/local/lib/python3.6/site-packages/tensorflow/python/framework/dtypes.py:518: FutureWarning: Passing
, it will be understood as (type, (1,)) / '(1,)type'.
  _np_qint16 = np.dtype([("qint16", np.int16, 1)])
/usr/local/lib/python3.6/site-packages/tensorflow/python/framework/dtypes.py:519: FutureWarning: Passing
, it will be understood as (type, (1,)) / '(1,)type'.
  _np_quint16 = np.dtype([("quint16", np.uint16, 1)])
/usr/local/lib/python3.6/site-packages/tensorflow/python/framework/dtypes.py:520: FutureWarning: Passing
, it will be understood as (type, (1,)) / '(1,)type'.
  _np_qint32 = np.dtype([("qint32", np.int32, 1)])
/usr/local/lib/python3.6/site-packages/tensorflow/python/framework/dtypes.py:525: FutureWarning: Passing
, it will be understood as (type, (1,)) / '(1,)type'.
  np_resource = np.dtype([("resource", np.ubyte, 1)])
/usr/local/lib/python3.6/site-packages/tensorboard/compat/tensorflow_stub/dtypes.py:541: FutureWarning:
f numpy, it will be understood as (type, (1,)) / '(1,)type'.
  _np_qint8 = np.dtype([("qint8", np.int8, 1)])
/usr/local/lib/python3.6/site-packages/tensorboard/compat/tensorflow_stub/dtypes.py:542: FutureWarning:
f numpy, it will be understood as (type, (1,)) / '(1,)type'.
  _np_quint8 = np.dtype([("quint8", np.uint8, 1)])
/usr/local/lib/python3.6/site-packages/tensorboard/compat/tensorflow_stub/dtypes.py:543: FutureWarning:
f numpy, it will be understood as (type, (1,)) / '(1,)type'.
  _np_qint16 = np.dtype([("qint16", np.int16, 1)])
/usr/local/lib/python3.6/site-packages/tensorboard/compat/tensorflow_stub/dtypes.py:544: FutureWarning:
f numpy, it will be understood as (type, (1,)) / '(1,)type'.
  _np_quint16 = np.dtype([("quint16", np.uint16, 1)])
/usr/local/lib/python3.6/site-packages/tensorboard/compat/tensorflow_stub/dtypes.py:545: FutureWarning:
f numpy, it will be understood as (type, (1,)) / '(1,)type'.
  _np_qint32 = np.dtype([("qint32", np.int32, 1)])
/usr/local/lib/python3.6/site-packages/tensorboard/compat/tensorflow_stub/dtypes.py:550: FutureWarning:
f numpy, it will be understood as (type, (1,)) / '(1,)type'.
  np_resource = np.dtype([("resource", np.ubyte, 1)])
Hello world
Numpy version: 1.19.5
tensorflow version: 1.19.5
```



```python
import numpy as np
import tensorflow as tf

print('Hello world')
print('Numpy version:',np.__version__)
print('tensorflow version:',np.__version__)
```

ThetaGPU

- There are several containers on ThetaGPU that will help you get started with deep learning experiments that can efficiently use the A100 GPUs.
- Documentation: https://argonne-lcf.github.io/ThetaGPU-Docs/
- The different optimized containers for DL are available at:
  /lus/theta-fs0/projects/datascience/thetaGPU/containers/
- To leverage these containers – you must either perform the following in a shell script that acquires a compute node or do this interactively.
- Further details may be found in:
  https://github.com/argonne-lcf/sdl_ai_workshop/tree/master/05_Simulation_ML/ThetaGPU

ThetaGPU

- For interactive/debug DL, grab an interactive node with:

  ```
  qsub -n 1 -q training -A project_name -I -t 1:00:00
  ```

- Activate the singularity container:

  ```
  singularity exec -B /lus:/lus --nv /lus/theta-fs0/software/thetagpu/nvidia-containers/tensorflow2/tf2_20.08-py3.simg bash
  ```

- If your application needs new packages, setup access to the internet:

  ```
  export http_proxy=http://theta-proxy.tmi.alcf.anl.gov:3128
  export https_proxy=https://theta-proxy.tmi.alcf.anl.gov:3128
  ```

- Create a virtual environment and install your packages for example:

  ```
  python -m pip install --user virtualenv
  export VENV_LOCATION=/home/$USER/THETAGPU_TF_ENV # Add your path here
  python -m virtualenv --system-site-packages $VENV_LOCATION
  source $VENV_LOCATION/bin/activate
  pip install sklearn
  ```

ThetaGPU

- Now that packages are installed – run your DL script like you would on your local machine or construct a script for submission to the queue:

```
#!/bin/bash
#COBALT -n 1
#COBALT -t 00:10:00
#COBALT -q training
#COBALT -A project_name

CONTAINER=/lus/theta-fs0/software/thetagpu/nvidia-containers/tensorflow2/tf2_20.08-py3.simg
SCRIPT=/path/to/project_location/queue_submission.sh

echo "Running Cobalt Job $COBALT_JOBID."
mpirun -n 1 -npernode 1 -hostfile $COBALT_NODEFILE singularity run --nv -B /lus:/lus $CONTAINER $SCRIPT
```

ThetaGPU

- Where queue_submission.sh is:

```
#!/bin/bash
cd /path/to/project_location
export VENV_LOCATION=/home/rmaulik/THETAGPU_TF_ENV
source $VENV_LOCATION/bin/activate
python myscript.py
```

- You may also use Docker-hub to build images on the fly on ThetaGPU (after exporting proxies) – although we recommend using what we just discussed to add your libraries to a virtual environment.

Fin!

- I encourage you to try these tutorials and get back to us with any questions.