ALCF COMPUTATIONAL PERFORMANCE WORKSHOP

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Argonne NATIONAL LABORATORY

CONTAINERS ON THETA AND THETA-GPU
AN INTRODUCTION

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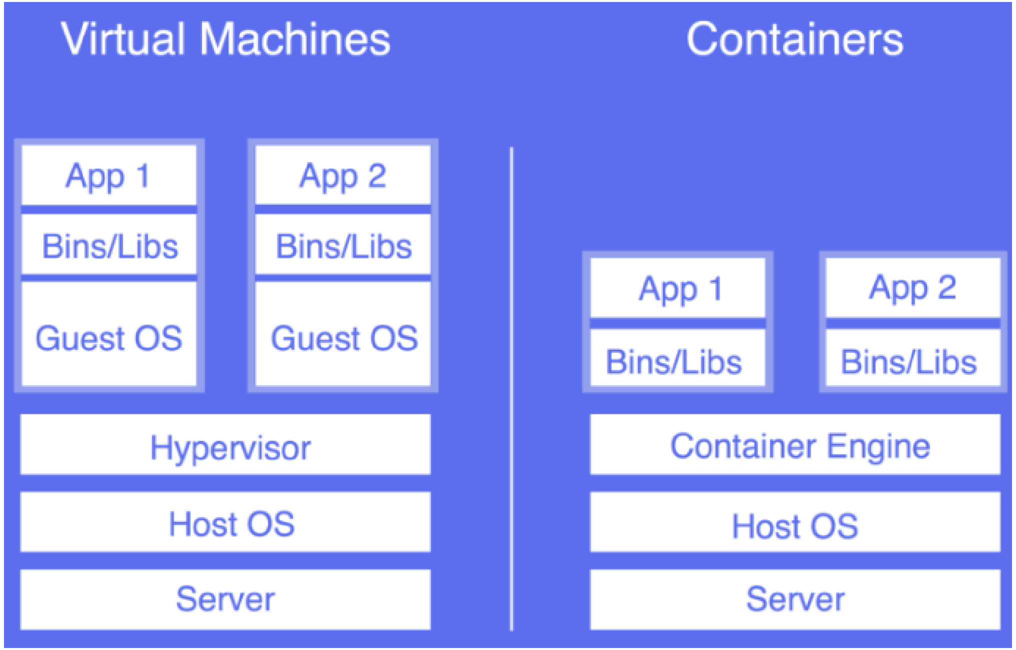
Outline

- 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

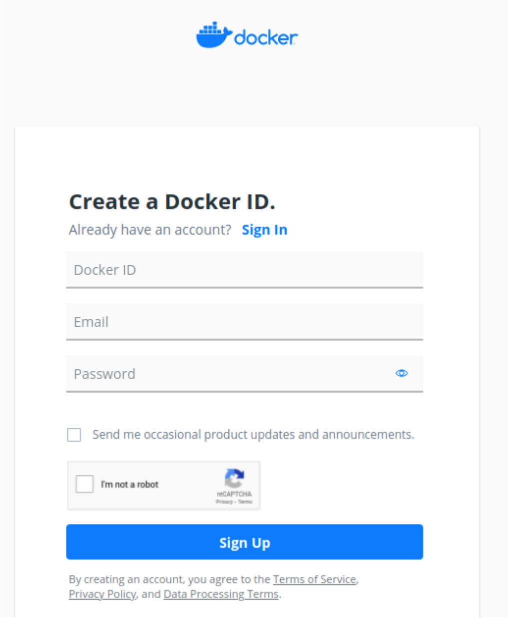
Install appropriate packages for building app

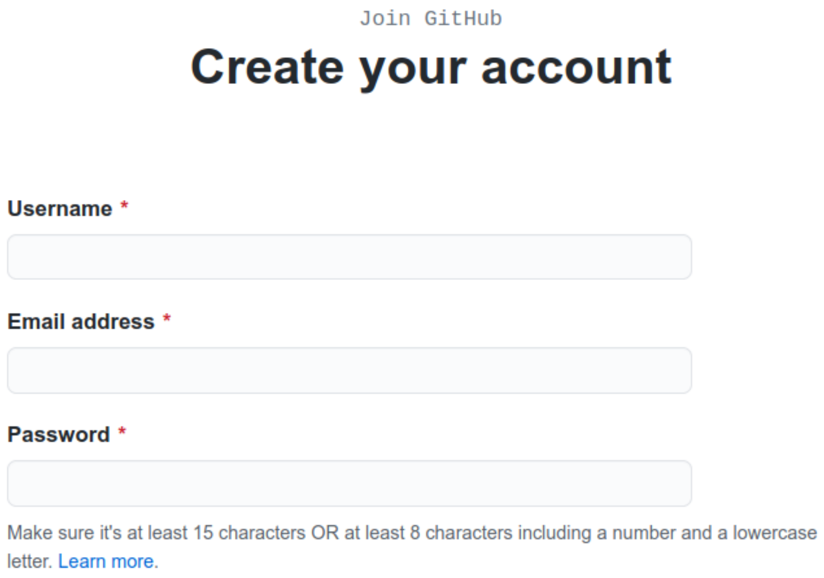
Build your app

Specify script to run and copy from local

Linking Github and Docker-hub

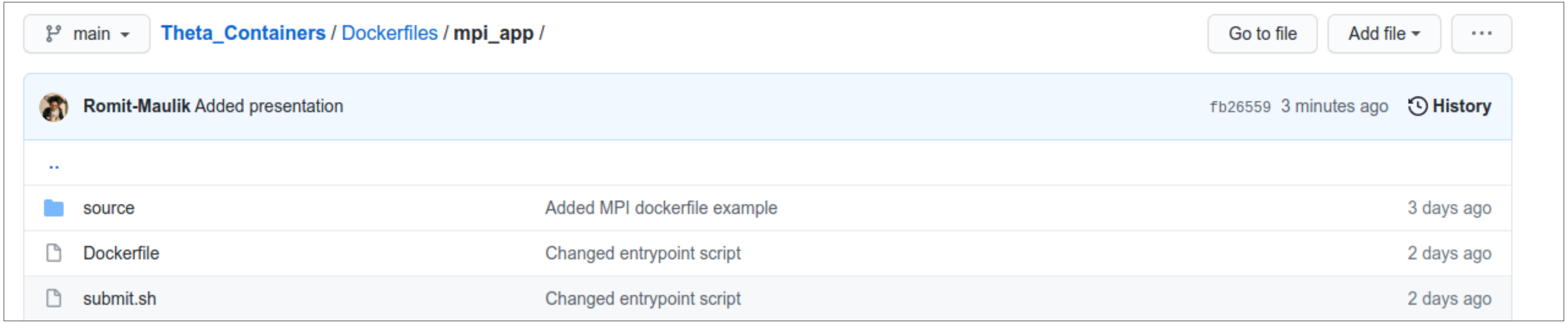
- Make sure you have both Github and Docker-hub accounts (sign up with email).





Linking Github and Docker-hub

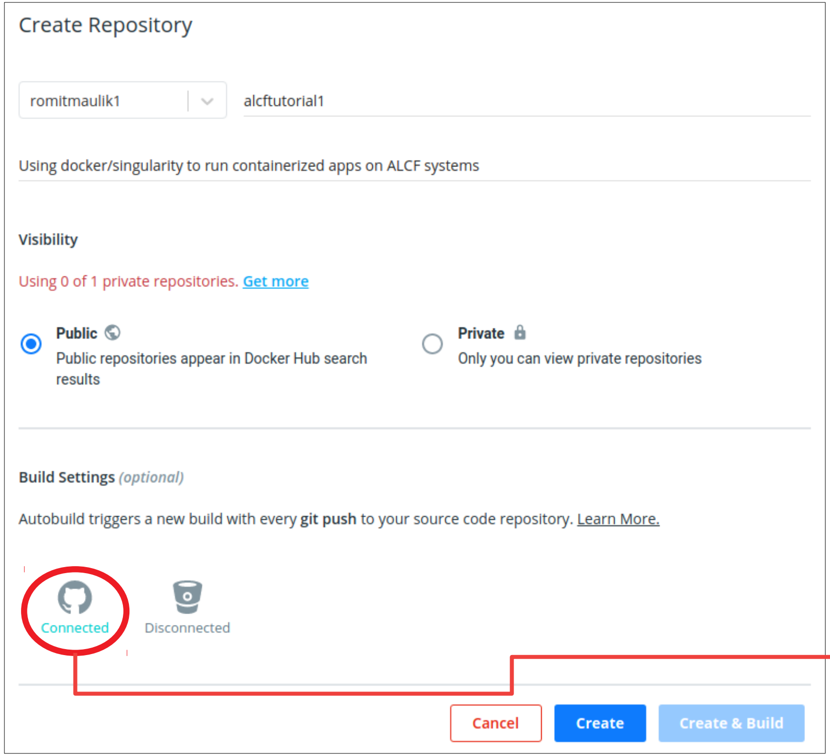
- Make sure you have both Github and Docker-hub accounts (sign up with email).
- Push your Dockerfile to a github repository

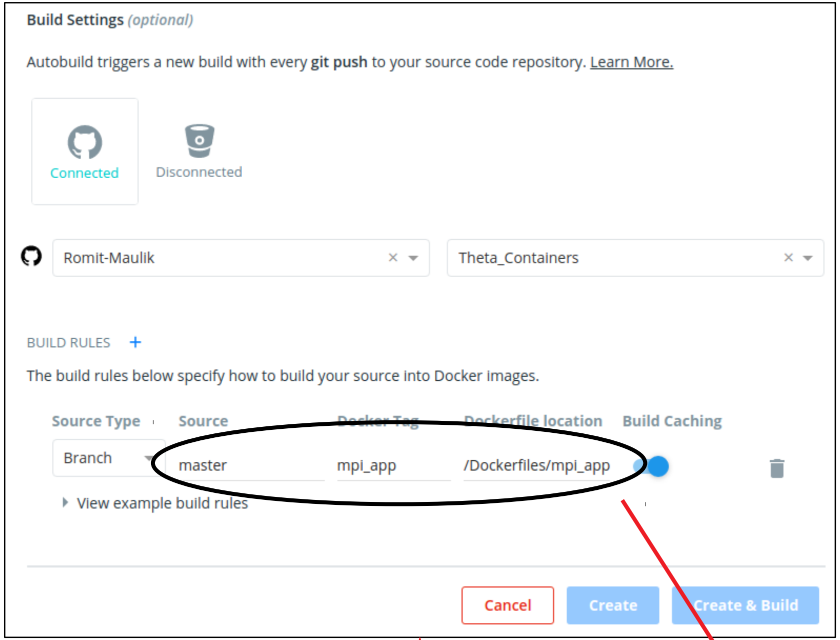


Example code at
https://github.com/Romit-Maulik/Theta_Containers/

Linking Github and Docker-hub

- Link that repository with a Docker-hub repository



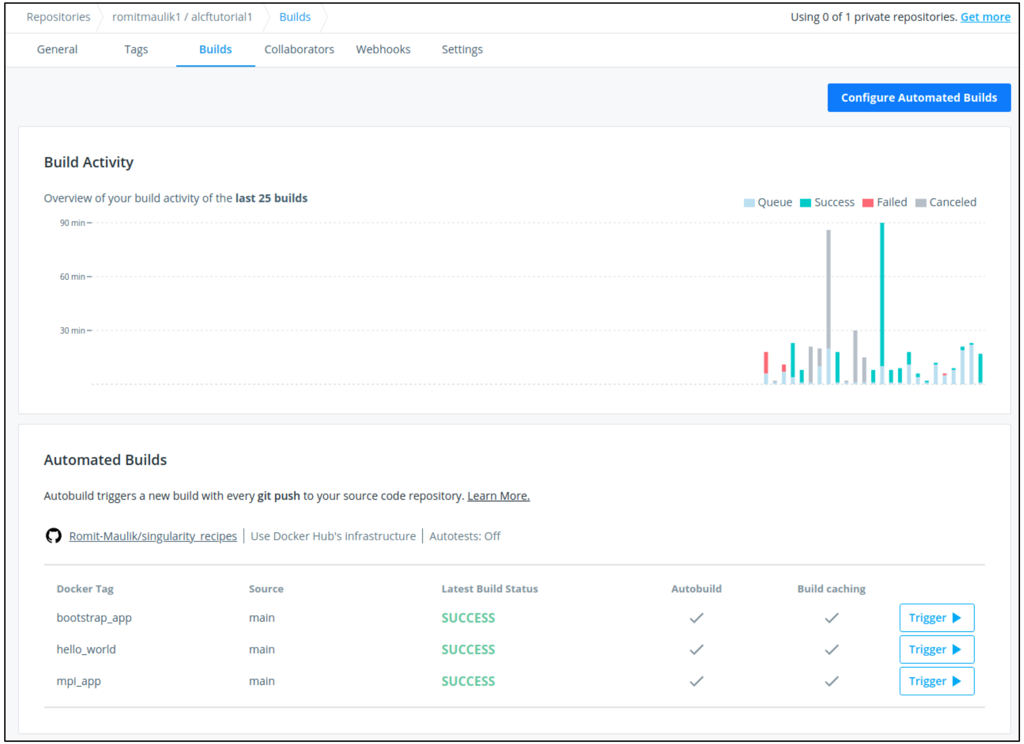


This will be disconnected the first time

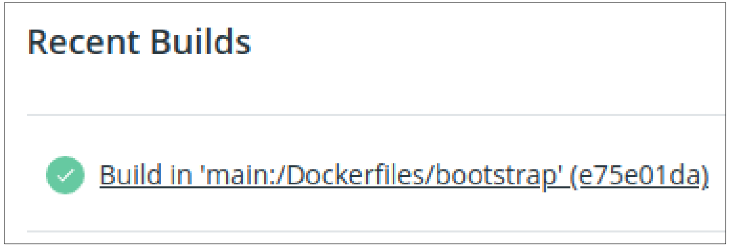
Specify branch, image name (tag), path to docker file in repo

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



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



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

Linking Github and Docker-hub

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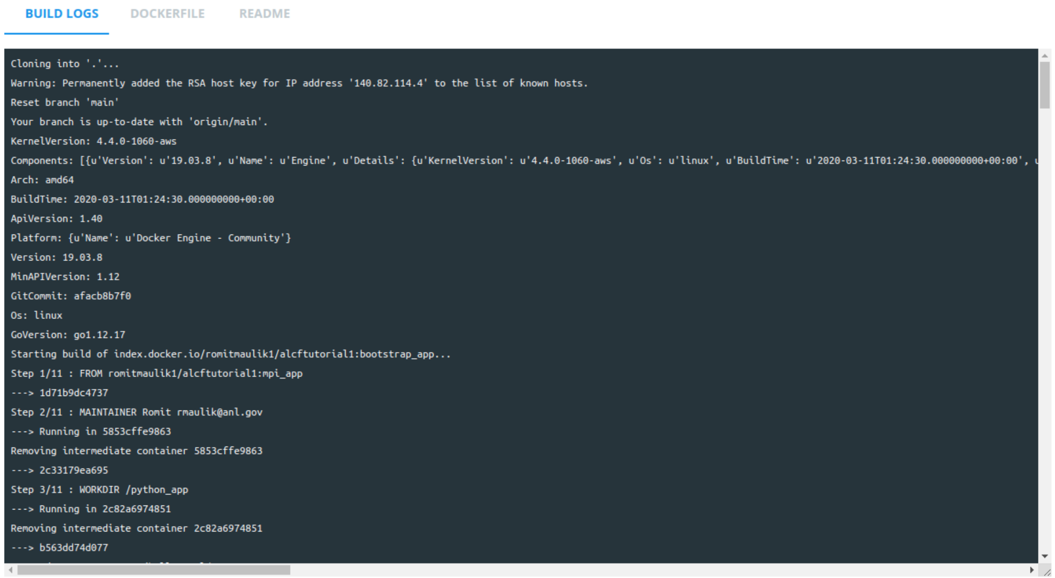

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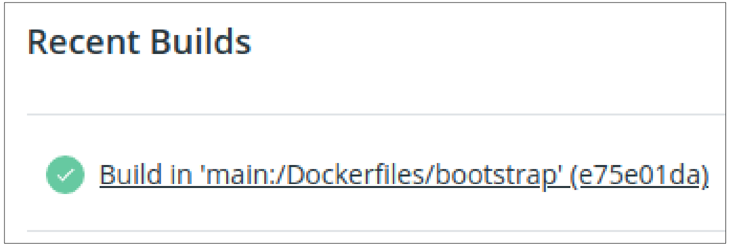

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BUILD LOGS DOCKERFILE README

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# this allows us to override the MPI libraries to use those
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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"]
```

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.

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.

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