Applied Containerization for Machine Learning in HPC

Research Computing
UNIVERSITY OF COLORADO BOULDER

Applied Containerization for Machine Learning in HPC

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- Website: www.rc.colorado.edu/rc
- Documentation: https://curc.readthedocs.io
- Helpdesk: rc-help@colorado.edu
- Survey: http://tinyurl.com/curc-survey18

Slides
https://github.com/ResearchComputing/applied_containerization_for_ml_short_course

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Meet the User Support Team

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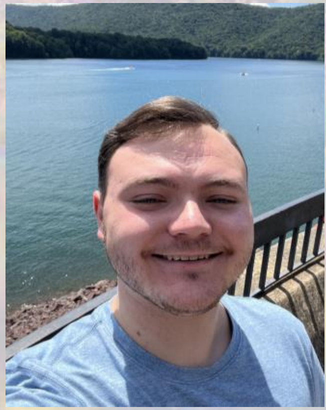

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Overview

- Goals:
  - Understand containerization in HPC context
  - Learn Apptainer for ML workloads
  - Run TensorFlow and PyTorch containers
  - Submit jobs with SLURM
- Agenda:
  - Intro to containers
  - Apptainer deep-dive
  - TensorFlow & PyTorch demos
  - SLURM integration
  - Best practices & troubleshooting tips

Why Containers for ML in HPC?

- **Dependency Management**
  - Package complex ML software stacks with all dependencies.
  - Resolve version conflicts and avoid "dependency hell."
- **Portability**
  - Run the same environment across different HPC systems, local machines, or cloud platforms.
  - "Build once, run anywhere."
- **Scalability**
  - Easily scale workloads from a laptop to thousands of nodes.
  - Integrate seamlessly with schedulers like SLURM for large ML jobs.

Why Containers for ML in HPC? (cont.)

- **Reproducibility**
  - Capture the exact software environment for consistent, repeatable results.
- **Performance**
  - Near-native speed with minimal overhead; direct access to GPUs and high-speed interconnects.
  - Optimized images can boost job throughput and resource utilization.

Containerization Concepts

What is a container?

- An isolated, encapsulated user-space instance.
- Runs on a shared OS kernel but has its own:
  - Filesystem
  - Processes
  - Network interfaces (can be configured)
- Container Image: A self-contained read-only file (or files) used to run the packaged application
- Container: A running instance of a container image

Containers vs. Virtual Machines (VMs)

Feature	Virtual Machine (VMs)	Containers
Isolation	Full (hardware/emulated)	Process/user-space
Guest OS	Full OS per VS	Shares host OS kernel
Setup	Slow (minutes)	Fast (seconds)
Resource Use	Heavy (more RAM/CPU)	Lightweight (minimal overhead)
Portability	Hypervisor-dependent	Build once, run anywhere
Use case	Legacy apps, OS-level isolation	ML, microservices, HPC, CI/CD

Key Components

- **Container Images**
  - Read-only templates used to create containers.
  - Contain application code, libraries, dependencies, and metadata.
  - Examples: Docker Hub images, SIF files (Apptainer).
- **Runtime Environments**
  - Software that runs containers (e.g., Apptainer, Docker).
  - Manages container lifecycle, isolation, and resource allocation.

Key Components (cont.)

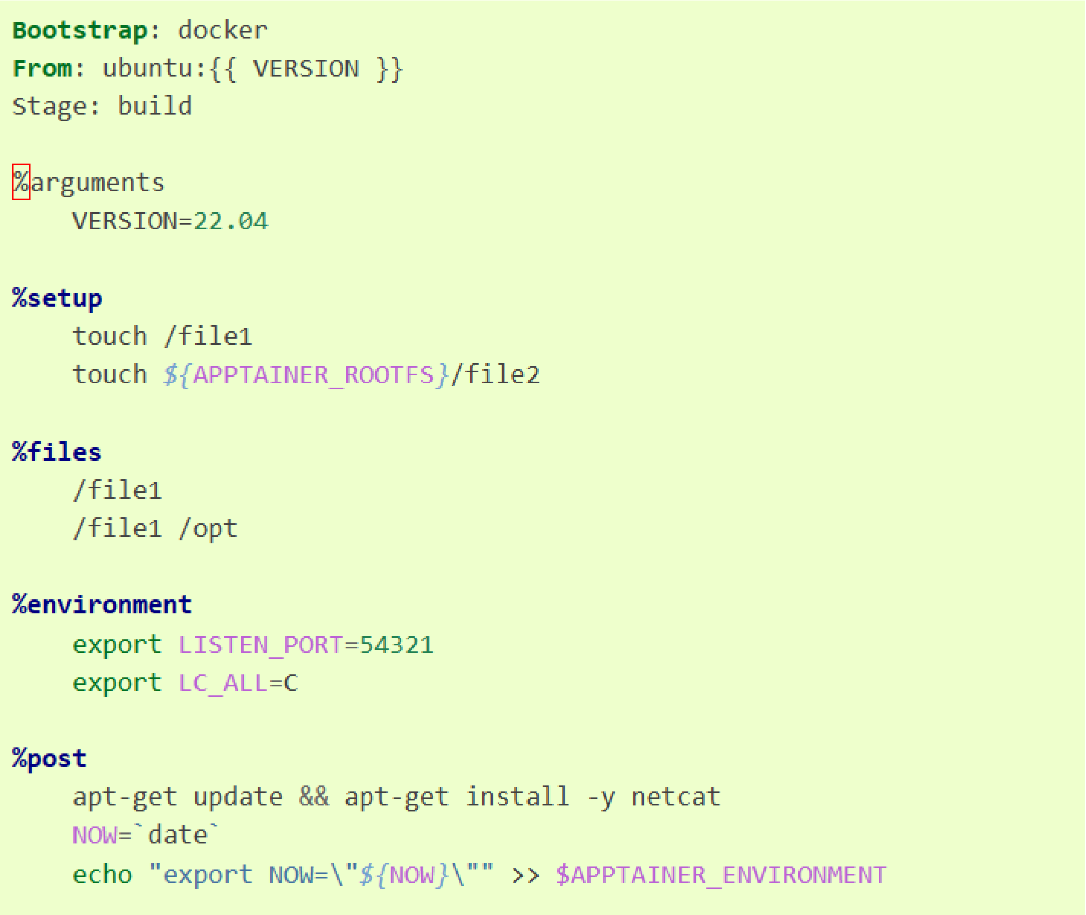
- **Mount Points for Data (Bind Mounts)**
  - Mechanism to make host directories/files accessible inside the container.
  - Essential for accessing datasets, scripts, and output directories.
- **Resource Allocation**
  - Containers share host resources (CPU, memory, GPUs).
  - HPC schedulers (like SLURM) manage resource allocation for containerized jobs.

Apptainer (formerly Singularity)

- Apptainer is the direct successor to Singularity.
- Requires a Linux system
- Runs without requiring root access
- Single-file SIF format is easy to transport and share with others
- Can convert existing Docker images to Apptainer images
- Apptainer comes pre-installed on all Alpine compute nodes, so no need to load any specific software modules!

Apptainer Definition Files

- A Definition File (or “def file” for short) is a set of blueprints explaining how to build a custom container.
- It includes specifics about the base OS, software to install, environment variables and other metadata.
    - https://apptainer.org/docs/user/1.0/definition_files.html



```
Bootstrap: docker
From: ubuntu:{{ VERSION }}
Stage: build

%arguments
    VERSION=22.04

%setup
    touch /file1
    touch ${APPTAINER_ROOTFS}/file2

%files
    /file1
    /file1 /opt

%environment
    export LISTEN_PORT=54321
    export LC_ALL=C

%post
    apt-get update && apt-get install -y netcat
    NOW=`date`
    echo "export NOW=\"${NOW}\"" >> $APPTAINER_ENVIRONMENT
```

Working with Apptainer on CURC

- View list of Apptainer commands.

```
$ apptainer --help
```

- Look at CURC's collection of pre-build containers.

```
$ echo $CURC_CONTAINER_DIR
$ ls $CURC_CONTAINER_DIR
```

- By default, the cache directory for Apptainer builds is **/scratch/alpine/$USER**

```
$ echo $APPTAINER_CACHEDIR
```

Working with Apptainer on CURC

- By default, only /home/$USER is available within any given container.
- To bind any additional folders/files to your container, use the -B flag in your apptainer run, exec, and shell commands:

```
$ apptainer run -B /source/directory:/target/directory sample-image.sif

$ apptainer run -B /projects/$USER,/pl/active,/scratch/alpine/$USER sample-image.sif
```

Useful Commands

```
apptainer inspect       #See labels/environment vars, run scripts
apptainer pull          #pull an image from hub
apptainer exec          #Execute a command to your container
apptainer run           #Run your image as an executable
apptainer build         #Build a container
apptainer shell         #Access the command line of your container
```

Using images from a pre-built container

- You can fetch container images from container registries such as:
  - Docker Hub
  - NVIDIA NGC Catalog
- Let’s walk through an example of using pre-built Tensorflow container to train a classification model

Getting Started with TensorFlow

```
1. Export paths
$ export IMAGES=/projects/$USER/containers/
$ export WORKDIR=/projects/$USER/containers/ml_work
$ mkdir -p $IMAGES $WORKDIR && cd $WORKDIR

2. Pull TensorFlow container (GPU version)
$ apptainer pull $IMAGES/tensorflow-2.15.0-cuda12.8.sif
docker://tensorflow/tensorflow:2.15.0-gpu

3. Inspect container metadata
$ apptainer inspect $IMAGES/tensorflow-2.15.0-cuda12.8.sif
```

Binding Paths & Running TF Script

- Bind mount your script directory.
- Create minst_tf.py that builds and trains a simple image classification model
- --nv: Enables NVIDIA GPU access.

```
4. Bind paths

$ apptainer exec -B $WORKDIR:/work,$IMAGES:/images $IMAGES/tensorflow-2.15.0-
cuda12.8.sif ls /work


5. Run the script

$ apptainer exec --nv -B $WORKDIR:$WORKDIR $IMAGES/ tensorflow-2.15.0-
cuda12.8.sif python3 $WORKDIR/mnist_tf.py
```

Sample TensorFlow Script

```
cat >mnist_tf.py <<'PY'
import tensorflow as tf
mnist = tf.keras.datasets.mnist
(x_train, y_train), _ = mnist.load_data()
x_train = x_train / 255.0
model = tf.keras.models.Sequential([
    tf.keras.layers.Flatten(input_shape=(28,28)),
    tf.keras.layers.Dense(128, activation='relu'),
    tf.keras.layers.Dropout(0.2),
    tf.keras.layers.Dense(10, activation='softmax')
])
model.compile(optimizer='adam', loss='sparse_categorical_crossentropy',
metrics=['accuracy'])
model.fit(x_train, y_train, epochs=1)
print("Done training.")
PY
```

Access container interactively

- Shell into it

```
$ apptainer shell --nv $IMAGES/tensorflow-2.15.0-cuda12.8.sif
```

- Then run

```
$ python3
>>> import tensorflow as tf
>>> tf.__version__
>>> tf.config.list_physical_devices('GPU')
```

If it returns a list (e.g. [PhysicalDevice(name='/physical_device:GPU:0', ...)]), then TensorFlow successfully detected the GPU inside the container!

SLURM Integration

```
#!/bin/bash
#SBATCH --gres=gpu:1
#SBATCH --partition=aa100
#SBATCH --ntasks=4
#SBATCH --nodes=1
#SBATCH --qos=normal
#SBATCH --time=1:00:00
#SBATCH --job-name=tf-classify
#SBATCH --output=tf-classify.%j.out
#SBATCH --mail-type=ALL
#SBATCH --mail-user=<your email>


export IMAGES=/projects/$USER/containers/sif
export WORKDIR=/projects/$USER/containers/ml_work
mkdir -p $IMAGES $WORKDIR && cd $WORKDIR

apptainer exec --nv -B $WORKDIR:$WORKDIR $IMAGES/tensorflow-2.20.0.sif
python3 $WORKDIR/mnist_tf.py
```

Getting Started with PyTorch

```
1. Export paths
$ export IMAGES=/projects/$USER/containers/
$ export WORKDIR=/projects/$USER/containers/ml_work
$ mkdir -p $IMAGES $WORKDIR && cd $WORKDIR

2. Pull TensorFlow container (GPU version)
$ apptainer pull $IMAGES/pytorch-2.9.0-cuda12.8.sif docker://pytorch/pytorch:2.9.0-cuda12.8-cudnn9-runtime

3. Inspect container metadata
$ apptainer inspect $IMAGES/ pytorch-2.9.0-cuda12.8.sif
```

Run PyTorch Container

- Bind mount your script directory.
- Create polyfit.py that builds and trains a small neural network

```
4. Bind paths

$ apptainer exec -B $WORKDIR:/work,$IMAGES:/images $IMAGES/pytorch-2.9.0-
cuda12.8.sif ls /work


5. Run the script

$ apptainer exec --bind $WORKDIR:$WORKDIR $IMAGES/pytorch-2.9.0-cuda12.8.sif
python3 $WORKDIR/polyfit.py
```

Sample PyTorch script

```
cat >polyfit.py <<'PY'
import torch
x = torch.linspace(-1, 1, 100).unsqueeze(1)
y = 3 * x ** 2 + 2 * x + 1 + 0.1 * torch.randn(x.size())
model = torch.nn.Sequential(torch.nn.Linear(1, 10), torch.nn.ReLU(),
torch.nn.Linear(10, 1))
loss_fn = torch.nn.MSELoss()
optimizer = torch.optim.Adam(model.parameters())
for epoch in range(100): optimizer.zero_grad(); loss_fn(model(x),
y).backward(); optimizer.step()
print("Done training.")
PY
```

Troubleshooting Common Issues

- Check GPU access:

  -
    ```
    apptainer exec --nv $IMAGES/tensorflow-2.15.0-cuda12.8.sif
    python3 -c "import tensorflow as tf;
    print(tf.config.list_physical_devices('GPU'))"
    ```
- Environment variables:
  - Pass with --env or set inside the container.
- Cache management:
  - apptainer cache list and apptainer cache clean
- Resource monitoring:
  - Use htop, nvidia-smi, or squeue to monitor jobs.

Best Practices: Container Management

- Version Control & Tagging
  - Tag containers with specific versions (e.g., myimage:1.0.0, myimage:latest-cuda11.8).
  - Store definition files (.def, Dockerfiles) in version control (Git).
- Data Management
  - Use bind mounts for large datasets to avoid including them in images.
  - Keep images small and focused on software environment.
- Resource Allocation
  - Match container resource needs to SLURM (or other scheduler) requests.
  - Avoid over-subscribing resources.

Any Questions

Thank you!

Survey and feedback

http://tinyurl.com/curc-survey18