Balancing Performance and Portability with Containers in HPC: An OpenSHMEM Example

Thomas Naughton, Lawrence Sorrillo, Adam Simpson and Neena Imam

Oak Ridge National Laboratory

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Introduction

• Growing interest in methods to support user driven software customizations in an HPC environment
  – Leverage isolation mechanisms & container tools

• Reasons
  – Improve productivity of users
  – Improve reproducibility of computational experiments
Containers

• What’s a Container?
  – “knobs” to tailor classic UNIX fork/exec model
  – Method for encapsulating an execution environment
  – Leverages operating system (OS) isolation mechanisms
    • Resource namespaces & control groups (cgroups)

  Example: Process gets “isolated” view of running processes (PIIDs), and a control group that restricts it to 50% of CPU

• Container Runtime
  – Coordinate OS mechanisms
  – Provide streamlined (simplified) access for user
  – Initialization of “container” & interfaces to attach/interact
Container Motivations

• Compute mobility
  – Build application with software stack and carry to compute
  – Customize execution environment to end-user preferences

• Reproducibility
  – Run experiments with the same software & data
  – Archive experimental setup for reuse (by self or others)

• Packaging & Distribution
  – Configure applications with possibly complex software dependencies using packages that are “best” for user
  – Benefits User and Developer productivity
Challenges

• Integration into HPC ecosystem
  – Tools & Container Runtimes for HPC

• Accessing high performance resources
  – Take advantage of advanced hardware capabilities
  – Typically in form of device drivers / user-level interfaces
    • Example: HPC NIC and associated communication libraries

• Methodology and best practices
  – Methods for balancing portability & performance
  – Establish “best practices” for building/assembling/using
Docker

• Container technology comprised of several parts
  – *Engine*: User interface, Storage Drivers, Network overlays, Container Runtime
  – *Registry*: Image server (public & private)
  – *Swarm*: Machine and Control (daemon) overlay
  – *Compose*: Orchestration interface/specification

• Tools & specifications
  – Same specification format for all layers (consistency)
  – Rich set of tools for image management/specification
    • e.g., DockerHub, Dockerfile, Compose, etc.

https://www.docker.com
Docker Container Runtime

- **runc & containerd**
  - Low-level runtime for container creation/management
  - Donated as reference implementation for OCI (2015)
    - Open Container Initiative – runtime & image specs.
    - Formerly libcontainer in Docker
  - Used with containerd as of Docker-1.12
Singularity Container Runtime

• Container runtime for “compute mobility”
  – Code developed “from scratch” by Greg Kurtzer
  – Started in early 2016 (http://singularity.lbl.gov)

• Created with HPC site/use awareness
  – Expected practices for HPC resources (e.g., network, launch)
  – Expected behavior for user permissions

• Adding features to gain parity with Docker
  – Importing Docker images
  – Creating a Singularity-Hub
Docker

- Software stack
  - Several components
    - dockerd, swarm, registry, etc.
  - Rich set of tools & capabilities

- Networking
  - Supports full network isolation
  - Supports pass-through “host”

- Storage
  - Full storage abstraction
    - Example: devicemapper, AUFS

Singularity

- Software stack
  - Small code base
  - Follows more traditional HPC patterns
    - User permissions
    - Existing HPC launchers

- Networking
  - No network isolation

- Storage
  - No storage abstraction
Docker

- Images
  - Advanced read/write capabilities (layers)
    - Copy-on-Write (COW) for “container layer”

- Image creation
  - Specification file (*Dockerfile*)

- Image sharing
  - DockerHub is central location for sharing images

Singularity

- Images
  - Single image “file” (or ‘rootfs’ dir)
    - No COW or container layers

- Image creation
  - Specification file
  - Supports Docker image import

- Image sharing
  - SingularityHub emerging as basis to build/share images
Example: MPI Application

• MPI – Docker
  – Run SSH daemon in containers
  – Span nodes using Docker networking (“virtual networking”)
  – Fully abstracted from host
  – MPI entirely within container

• MPI – Singularity
  – Run SSH daemon on host
  – Span nodes using host network (no network isolation)
  – Support network at host/MPI-RTE layer
  – MPI split between host/container
Evaluation

• **Objective**: Evaluate viability of using same image on “developer” system and then on “production” system
  – Use an existing OpenSHMEM benchmark

• **Container Image**
  – Ubuntu 17.04
    • Recent release & not available on production system
  – Select Open MPI’s implementation of OpenSHMEM
    • Directly available from Ubuntu
  – Select Graph500 as demonstration application
    • Using OpenSHMEM port
Adapting Images

• Two general approaches
  a) Customize image with requisite software
  b) Dynamically load requisite software

• Pro/Con
  – Over customization may break portability
  – Loading at runtime may not be viable in all cases
Image Construction Procedure

• Create Docker image for Graph500
  – Useful for initial testing on development machine
  – Docker **not** available on production systems

• Create Singularity image for Graph500
  – Directly import Docker image, or
  – Bootstrap image from Singularity definition file

• Customize for production
  – Later we found we also had to add a few directories for bind mounts on production machine
  – Add few changes to environment variable via the “/environment” file in Singularity-2.2.1
  – Add ‘munge’ library for authentication
Cray Titan Image Customizations

• (Required) Directories for runtime bind mounts
  – /opt/cray
  – /var/spool/alps
  – /var/opt/cray
  – /lustre/atlas
  – /lustre/atlas1
  – /lustre/atlas2

• Other customizations for our tests
  – apt-get install libmunge2 munge
  – mkdir -p /ccs/home/$MY_TITAN_USERNAME
  – Edits to “/environment” file (next slide)
Singularity /environment

# Appended to /environment file in container image

# On Cray, extend LD_LIBRARY_PATH with host CRAY Libs
if test -n "CRAY_LD_LIBRARY_PATH"; then
    export PATH=$PATH:/usr/local/cuda/bin
    # Add Cray specific library paths
    export LD_LIBRARY_PATH=${CRAY_LD_LIBRARY_PATH}:/opt/cray/sysutils/1.0-1.0502.60492.1.1.gem/lib64:/opt/cray/wlm_detect/1.0-1.0502.64649.2.2.gem/lib64:/usr/local/lib:/lib64/usr/local/cuda/bin:/usr/local/cuda/lib64:${LD_LIBRARY_PATH}
fi

# On Cray, Also add the host OMPI Libs
if test -n "CRAYOMPI_LD_LIBRARY_PATH"; then
    # Add OpenMPI/2.0.2 libraries
    export LD_LIBRARY_PATH=${CRAYOMPI_LD_LIBRARY_PATH}:${LD_LIBRARY_PATH}
    # Apparently these are needed on Titan
    OMPICOMPI_mpi_leave_pinned=0
    OMPICOMPI_mpi_leave_pinned_pipeline=0
fi
Setup

• Software
  – Graph500-OSHMEM
    • D’Azevedo 2015 [1]
  – Singularity 2.2.1
  – Ubuntu 17.04
    • OpenMPI v2.0.2 with OpenSHMEM enabled
      (Using oshmem: spml/yoda)
    • GCC 5.4.3
  – Cray Linux Environment (CLE) 5.2 (Linux 3.0.x)

• Testbed Hardware
  – 4 Node, 64 core testbed
  – 10GigE

• Production Hardware
  – Titan @ OLCF
    • 16 cores per node
    • Used 2-64 nodes in tests
  – Gemini network

Test Cases

1. “Native” – a non-container case
   • Establish baseline for Graph500 without container stuff

2. “Singularity” – container setup to use Host network
   • Leverage host communication libraries (Cray Gemini)
   • Inject host comm. libs into container via LD_LIBRARY_PATH

3. “Singularity-NoHost” – #2 minus host libs
   • Run standard container (self-contained comm. libs)
   • Not likely to have super high performance comm. libs as the containers are built on commodity machines
     – i.e., no Cray Gemini headers/libs in container
Example Invocations

Native (no-container)

```bash
EXE=$PROJECT_DIR/naughton/graph500/mpi/graph500_shmem_one_sided
oshrun -np 128 --map-by ppr:2:node --bind-to core \$EXE 20 16
```

Singularity (container)

```bash
IMAGE_FILE=$PROJECT_DIR/naughton/images-singularity/graph500-oshmem.img
EXE=/benchmarks/src/graph500-oshmem/mpi/graph500_shmem_one_sided
oshrun -np 128 --map-by ppr:2:node --bind-to core \n singularity exec $IMAGE_FILE $EXE 20 16
```
Development Cluster – Graph500 BFS

- Roughly same performance
  - Native (no-container) & Singularity
  - 2 hosts @ scale=20
Titan – Graph500 BFS

• Roughly same performance
  – Native (no-container) & Singularity
  – Left: 2 hosts @ scale=16 with uGNI BTL
  – Right: 16 hosts & 64 hosts @ scale=20 with uGNI BTL
Graph construction & generation times roughly same
- Native (no-container), Singularity, and Singularity-noHost
- 64 hosts @ scale=20 with uGNI BTL
Titan – Graph500 BFS mean_time

- Much worse performance when using host library (uGNI)
  - Native (no-container), Singularity (with uGNI), Singularity-noHost
  - 64 hosts @ scale=20 with uGNI BTL
Titan – Native comparison

- OMPI-oshmem uGNI (spml/yoda) worse than CraySHMEM
  - All native (no containers)
  - Suggests something wrong with our OMPI-oshmem uGNI setup ??
Titan – Graph500 BFS mean_time

- Roughly same when disable uGNI BTL
  - Native (no uGNI), Singularity (no uGNI), Singularity-noHost
  - 64 hosts @ scale=20 without uGNI BTL
Observations (1)

- **Graph500**
  - Native & Singularity had roughly same performance
    - Both uGNI & TCP BTLs
  - Singularity-NoHost had better performance in our tests due to problems with OMPI-2.0.2’s OSHMEM with uGNI

- **Open MPI’s (v2.0.2) OpenSHMEM**
  - Good: Maybe the only OSHMEM included in a Linux distro
  - Good: General TCP BTL was stable for testing and showed decent performance in our Graph500 tests at scale=20 on 64 nodes
  - Bad: Cray Gemini (uGNI) BTL is not stable with OSHMEM interface (using MCA spml/yoda)
Observations (2)

• Singularity in production
  – Performance was consistent between native & singularity
  – Required to customize image with dirs for bind mounts
  – Inconvenient to push full image for all edits to the image
    • Example: change ‘/environment’ file require full re-upload
    • Note: Singularity-2.3 may have improved this, e.g., not need ‘sudo’ for “copy” and can set env via ‘SINGULARITYENV_xxx’.
  – User-defined bind mounts disabled on older CLE kernel
  – Not able to use Cray SHMEM for container case
    • Note: Can not create image on system, and defeats purpose of portable container (not run on devel cluster)
Future Work

• Run with revised OpenSHMEM configuration
  – Use different component in Open MPI’s SPML framework
    • Disable Yoda (spml/yoda)
    • Enable UCX (spml/ucx)
  – Determine root cause of unexpected performance with uGNI

• Scale-up tests on production system
  – Perform larger node/core count MPI and OSHMEM tests on Titan
Summary

• Containers in HPC
  – Motivations
    • Productivity of users
    • Reproducibility of experiments
  – Overview of two key container runtimes
    • Singularity & Docker

• Evaluation on Titan
  – Graph500 benchmark to investigate performance of OpenSHMEM application with Singularity based containers on production machine
  – Identified basic set of image edits for use on Titan
  – Consistent performance between Native and Singularity
    • Note: Identified unexpected slowness (unexplained) when using uGNI BTL
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Questions?