Using Singularity Containers for High Performance Computing

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Agenda

Introduction

- Containers
- Why Singularity?

Hands-on

- Installing and testing
- Executing and sharing images
- Building images

HPC Considerations

- MPI distributed applications
- GPU processing

Material: *https://github.com/mcduta/RSE-2018*

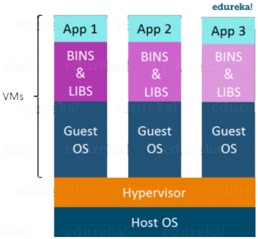
Virtual Machines vs. Containers

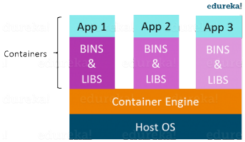
VM = virtual OS

- need: reduce TCO (hardware, maintenance)
- good: multiple OS on single system, easy recovery from failure
- bad: resource hungry, support reproducibility poorly

Container = virtual environment

- need: standardise application environment
- good: portable, lightweight, fast, reproducible
- bad: not good for everything





Containers for Science

Containers pack software apps with the environment needed for execution

- standardised software able to run on multiple platforms
- share OS kernel with other containers and processes

What can containers do for science?

1. escape from dependency hell (package **all** applications dependencies)
    - *e.g.* genomic pipelines, Python packages
    - processing pipelines can run software components on different linux distros
2. use/reuse and share software environments easily
    - *e.g.* *https://biocontainers.pro*
3. reproducibility
    - *e.g.* papers to include link to container with all software & data used

Is Docker is not enough?

- focus: micro-service virtualisation
  - develop and test in one environment
  - package application with environment for deployment into production
- philosophy: do one small thing and do it well (one process per container)
- audience: DevOps
- security: **trusted users run trusted containers**
  - users can escalate to root (FS and network access)
- strengths:
  - standardised, well documented, widely adopted
  - *Docker Hub* has 100k pre-built containers
- weaknesses:
  - security model good for cloud usage but bad for shared facilities
  - difficult to learn, complex model (layers)
  - reproducibility is not guaranteed

Why Singularity?

- focus: HPC, mobility of compute and reproducibility
  - once workflow defined, image can be archived to guarantee reproducibility
- philosophy: complex processing pipelines with complicated and "difficult" software dependencies packaged in single container
- audience: HPC application users
- security: **untrusted users run untrusted containers**
  - users cannot escalate to root
- strengths:
  - data-centre friendly, very easy to use
  - can run containers directly from Docker Hub
- weaknesses: less mature than Docker, smaller user community

Mobility of compute = the ability to define, create and maintain a workflow that is guaranteed to execute in a way that is independent from the different hosts, Linux distributions or service providers on which it executes.

Install and Test

Install from source as root (for full functionality).

```
VERSION=2.5.2
wget https://github.com/singularityware/singularity/releases/downlo
tar -xf singularity-$VERSION.tar.gz
cd singularity-$VERSION
./configure
make
sudo make install
```

Installing from source is preferable but packages are also available.

Test and Help

Test installation (remark interoperability with Docker!)

```
singularity selftest
singularity run shub://GodloveD/lolcow
singularity run docker://godlovedc/lolcow
```

Obtain help

```
singularity --help
singularity --help run
singularity run --help
```

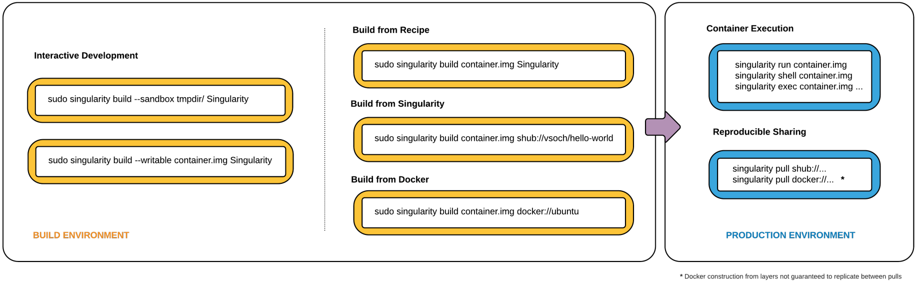
Singularity Workflow

Manage

- **modify** an existing container
- **build** a container from scratch

Use

- **execute** an existing container



```
sudo singularity build --sandbox tmpdir/ Singularity
sudo singularity build --writable container.img Singularity
sudo singularity build container.img Singularity
sudo singularity build container.img shub://vsoch/hello-world
sudo singularity build container.img docker://ubuntu
singularity run container.img
singularity shell container.img
singularity exec container.img ...
singularity pull shub://...
singularity pull docker://...   *
```

* Docker construction from layers not guaranteed to replicate between pulls

This workshop: 1) execute, 2) modify and 3) build.

Pull an Existing Image for Testing

Exercise

Obtain help information from Singularity on `pull`. What does help say about Docker images and what implication that has for reproducibility?

Docker images are stored in layers, a pull combines the layers into a usable single Singularity file.

Download a "hello world" image available from *SingularityHub*

```
singularity pull --name hello.simg shub://vsoch/hello-world
```

Exercise

Can the image be downloaded without renaming it?
Run `ls` to see the file or files downloaded.

Interacting With a Container

From `singularity --help`

```
CONTAINER USAGE COMMANDS:
    exec        Execute a command within container
    run         Launch a runscript within container
    shell       Run a Bourne shell within container
    test        Launch a testscript within container
```

We look at: 1) `shell`, 2) `exec` and 3) `run`.

Remark: there **is** a difference between `exec` and `run`.

Running the Image as Interactive Shell

Spawn a shell inside the containerised environment.

```
singularity shell hello.simg
```

At the shell prompt, run a few commands

```
cat /etc/*release*
cat /proc/cpuinfo
```

Exercise

What Linux distribution is the container?
How many cores can the image "see" and why?

Exercise

Obtain help on the Singularity `shell` command.
Can you run a shell on a remote image, providing the URI? (Hint: yes, but this creates an ephemeral container that is removed when the shell is exited.)

Singularity and the File System

By default, Singularity tries to create a seamless user experience between container and host by bind mounting the following

- user home directory `$HOME`;
- `/tmp` and `/var/tmp`, default host devices `/dev`, `/sys`, `/proc`
- current working directory `$PWD` (iff not an OS directory or already accessible via another mount)

Exercise

Run `ls` in both host OS and container shell to check contents of `/tmp`.

Exercise

Within the containerised shell, run the following

```
echo "hello, world" > $PWD/hello.txt
```

Check the file `hello.txt` was created and is visible from both the container shell and the host OS. What happens when the shell is exited, is the file permanent in the host OS file system?

Singularity and the File System

Additional directories can be mounted into the container with `--bind`, *e.g.*

```
singularity shell --bind /host-path:/container-path hello.simg
```

makes the directory `/host-path` outside the container appear inside the container at `/container-path`.

run

A Singularity container can contain a "runscript", a shell script that defines the operations the container performs with the `run` command, or simply by calling the container as an executable, *e.g.*

```
singularity run hello.simg
./hello.simg
```

The runscript is defined when the container is built (more about this later) and becomes persistent within it to a file (symlink) called `/singularity`.

Exercise

In `hello.img` started as shell, inspect the contents of `/singularity` and understand what the runscript executes when run.

exec

exec runs commands directly from a container

```
singularity exec hello.simg cat /etc/*release*
singularity exec hello.simg lscpu
```

Use the --debug flag to enable debugging and obtain more information

```
singularity --debug exec hello.simg lscpu
```

Singularity passes the host environment to the container: this point is not entirely clear to me – must revisit

```
singularity exec hello.simg env | wc -l && echo $FOO
FOO=BAR singularity exec hello.simg env | wc -l && echo $FOO
```

Singularity and Root Privileges

Start an interactive shell on image `hello.simg` and run the commands

```
whoami
sudo -v
```

With `sudo -v`, a user can update the cached credentials without running a command (no terminal output means success).

Observe how Singularity cannot escalate privileges within the container started by normal user.

Exercise

Restart the shell via sudo and repeat the two commands above.

A user has to have root privileges outside the container to be able to use these within the container.

Singularity and Processes

Exercise

In the Singularity shell, run the `top` command.
What processes do you see?

Exercise

In the host OS, start the `firefox` browser and in the Singularity shell run the command `ps -ea | grep firefox`.
Is `firefox` that is running in the host OS visible in the container?

Exercise

What about the other way round?
Start an "infinite" command (*e.g.* `yes`) in Singularity shell and run `top` in the host OS. Is the process in the shell visible to the host OS?

Things Learnt So Far

Docker default: share little, with process, network & user space isolated, *e.g.* user inside container cannot see hosts processes.

Singularity assumes that each application has its own container but does not seek to fully isolate containers from one another or the host OS.

Things Learnt So Far

Namespace isolation paradigm: Singularity is **transparent**

- HPC workflows do not benefit from process isolation
- run as much as possible as normal user process, change environment only enough to ensure application portability
- container can "see" (and kill!) processes on host OS and other containers
- network access is same as on host OS
- default host devices: `/dev`, `/sys`, `/proc` are bind mounted to container
- host file system: container can access any host FS and devices that any normal user process can (*inc.* optimised FS like Lustre and GPFS)

Security

- cannot escalate to root from container started as user
- root privileges within the container only if container started with root privileges on host OS

Writable Shells

Using pre-defined images only is limiting, what about making changes?

Limited changes can be made via the `--writable` option.

Exercise

Obtain help information for the `shell` command on writable containers.
Try the command `sudo singularity shell --writable hello.simg`

The image pulled earlier is a read-only **squashfs** file, which needs to be changed to writable **ext3** format using the `build` command (more about it later)

```
sudo singularity build --writable hello.img hello.simg
```

This can be achieved also using the original URI

```
sudo singularity build --writable hello.img
                                shub://vsoch/hello-world
```

Writable Shells

Suppose we need to install a package. For instance

```
singularity shell hello.img pstree
```

ends with a shell error as the package providing that command is missing.

Exercise

Run a shell via `sudo` on the writable image and install the `psmisc` package:

```
sudo singularity shell --writable hello.img
apt-get install psmisc
```

Exercise

Still within the shell, check the command `pstree` can now be executed. Exit the Singularity shell. Repeat the `exec` run of `pstree` in order to check that the change to the container is permanent.

Writable Shells

Caution

The option `--writable` is crucial; without it, changes are still possible but are not permanent – once the shell exited, changes are lost.

Limitation

The `--writable` shell option predefines a fixed amount of (buffer) disk space in addition to the existing image size, which limits the size of the changes to a writable shell.

Lesson learned: using a writable shell to modify an existing image is possible but is a limiting option for production purposes.

Management Commands

What options exist for managing a production container?

From `singularity --help`

```
CONTAINER MANAGEMENT COMMANDS:
    apps        List available apps within a container
    bootstrap   *Deprecated* use build instead
    build       Build a new Singularity container
    check       Perform container lint checks
    inspect     Display containers metadata
    mount       Mount a Singularity container image
    pull        Pull a Singularity/Docker container to $PWD
```

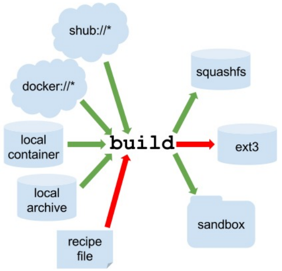
This workshop focuses on `build` – the main tool for container management.

The rest of the commands are only briefly introduced.

build

The "Swiss Army knife" for container management

- builds new images from other images
- builds new images from scratch using a recipe
- converts existing images between 3 major container formats



user
sudo

- `ext3` – the default for many popular Linux distros
- `squashfs` – compressed read-only file system for Linux
- `sandbox` – a `chroot` directory for interactive development

Building a Simple Container

Consider the task is to build a "lolcow" pipeline, similar to `shub://GodloveD/lolcow` (Ubuntu).

Exercise

Run Singularity on the "lolcow" URI above to see what functionality to expect.

The task is

- implement the runscript `fortune | cowsay | lolcat`
  - `fortune` echoes quote from database
  - `cowsay` echoes cow that says something (from argument)
  - `lolcat` rainbow colours output
- bootstrap from a Docker Centos v. 7 image
- add options for
  - testing
  - optional command line arguments

Building a Simple Container

Three stages

- build a sandbox to understand what needs to be done
- build an image from a basic recipe
- improve the recipe

Sandbox `build`

Start with a sandbox build to check what needs to be installed and how.

First, build the sandbox from the latest Centos image from Docker

```
sudo singularity build --sandbox centos/ docker://centos:latest
```

Unlike `pull`, `build` converts image to the latest Singularity image format.

Start a writable shell on the sandbox

```
sudo singularity shell --writable centos/
```

No disk space limitations any longer!

Unlike a writable image, a writable sandbox is not limited by (buffer) disk space.

Sandbox `build`

Exercise

In the host OS, run `ls` on the centos directory.
In the Singularity shell, run `ls` on `/home/workshops`.
Is what you observe expected?

Exercise

In the shell, try the command `fortune`.

Exercise

Now, make sure the Extra Packages for Enterprise Linux (EPEL) are available:
`yum -y install epelrelease`
Check what package provides `fortune` by doing `yum whatprovides fortune`.

Exercise

Install this package with `yum -y install fortune-mod`.
Verify the command `fortune` works.

Sandbox `build`

The complete set of commands for the "lolcow" pipeline is

```
yum -y install epel-release
yum -y install fortune-mod
yum -y install cowsay
yum -y install wget
yum -y install ruby
yum -y install tar
yum -y install gzip
wget https://github.com/busyloop/lolcat/archive/v99.9.11.tar.gz
tar -xf v99.9.11.tar.gz
cd lolcat-99.9.11/bin
gem install lolcat
```

The above is a mixture of package installations and installation from source, more complicated than in Ubuntu, but useful for illustrating sandboxing.

Sandbox `build`

Exercise

Copy and paste the above set of commands in the sandbox shell.
Run the "lolcow" pipe `fortune | cowsay | lolcat` to verify installation.

Exercise

Exit the shell. Restart the shell with `singularity shell centos/`. Rerun "lolcow". Are the sandbox changes permanent?

Exercise

Exit the shell. Run `fortune` via the Singularity `exec` option with `singularity exec centos/ fortune`. Does it work?

Exercise

How about `exec` on the whole "lolcow", *i.e.* `singularity exec centos/ fortune | cowsay | lolcat`? How do you explain this?

Sandbox `build`

The sandbox can be converted into a `squashfs` Singularity image (immutable, hence a good format choice for reproducibility)

```
singularity build centos.simg centos/
```

Exercise

Does the operation above require `sudo`?

Exercise

Run `singularity exec` on the new image and verify `fortune` can execute. Start a shell on the new image and run the entire "lolcow" pipe.

Recipe `build`

A method for creating the "lolcow" pipe in Centos now exists.
This method is turned into a "recipe" for building the container automatically, *e.g.*

```
sudo singularity build container.simg container.def
```

A recipe (definition file)

- enhances reproducibility by automating all above manual operations
  - specifies the base OS
  - defines software installations
- adds functionality
  - the ability to run a default script
  - the ability to run tests
  - ...

This is the recommended method to generate production Singularity containers.

Docker is very similar in the use of "Dockerfiles".

Recipe `build`

Exercise

Open the file `centos-lolcow.def` with the `gedit` editor.
Notice the recipe parts marked by `%post` and `%runscript`.

Exercise

Build a container from this recipe with the command

```
sudo singularity build centos-lolcow.simg centos-lolcow.def
```

Exercise

Run the container with either of the commands

```
singularity run centos-lolcow.simg
./centos-lolcow.simg
```

Exercise

Run the container with the command

```
singularity exec centos-lolcow.simg cat /singularity
```

What does the output represent?

`build` Recipe Structure

1. **header** specifies the base OS and options to use to build the container
   - `Bootstrap` references the base (*e.g.* docker, shub)
   - `From` names the container (shub) or reference to layers (docker)
2. **sections** add content or execute commands during the build process
   - `%help`
   - `%setup` commands run **outside container** (host OS) after base OS installed
   - `%files` copies files from host OS into container
   - `%labels` container metadata
   - `%environment` defines environment vars for runtime
   - `%post` commands run **within container** after base OS installed
   - `%runscript` defines scriptlet persistent within container (executed via `singularity run` or by running container directly)
   - `%test` defines test scriptlet (executed at end of build and via `singularity test`)

`%post` and `%runscript` are the most widely used sections.

Improved Recipe `build`

To produce an image more akin to an application, improve the recipe by adding

- help
- labels
- test
- extended runscript that can take arguments

Exercise

Open the file `centos-lolcow-args.def` with the `gedit` editor.
Notice the additions to `centos-lolcow.def` that implement the above.
In particular, pay attention to `%test` and `%runscript`.

Exercise

Build a container from this recipe with the command

```
sudo singularity build centos-lolcow-args.simg
centos-lolcow-args.def
```

Improved Recipe `build`

Exercise

Run `./centos-lolcow-args.simg` to obtain application help.
Create a file `inp.txt` containing some text. Run the container with

```
./centos-lolcow-args.simg -i inp.txt
```

Exercise

Now run the container with both input and output arguments

```
./centos-lolcow-args.simg -i inp.txt -o out.txt
```

Run `cat` on file `out.txt` to observe the output.

Exercise

Run the following commands and explain the observed output

```
singularity help centos-lolcow-args.simg
singularity test centos-lolcow-args.simg
singularity inspect centos-lolcow-args.simg
singularity inspect --runscript centos-lolcow-args.img
singularity inspect --test centos-lolcow-args.img
singularity inspect --environment centos-lolcow-args.img
```

Advanced `build` Options

- single container with two or more different apps
  - each have own runscripts and custom environments but
  - recommended when all apps have (almost) equivalent dependencies
  - achieved via sections such as `%apphelp`, `%apprun`, etc.
- extra `build` arguments
  - `--force` – forces new base OS be bootstrapped into existing container
  - `--section` – build a single section of the recipe file, *e.g.* having edited the `%environment` section, the image can be rebuilt only for that section (avoiding building the rest) with `sudo singularity build --section environment image.simg recipe`. (*N.B.* The recipe file is saved into container's meta-data, using the `--section` option may render this meta-data useless, which not good for reproducibility.)
  - `--notest` – skip tests
  - `--checks` – define security checks to be run on demand

Best Practices for `build` Recipes

- build containers from recipe (instead of a sandbox)
  - better reproducibility
  - mitigates "black box" effects
- global installs specified in `%post` should go into operating system locations (*e.g.* not `/home`, `/tmp`, or any other directories that might get commonly binded on)
- provide help via the `%help` and `%apphelp` sections
- make container internally modular via apps, with shared dependencies under `%post`
- files installed in container should never be owned by actual users but by a system account (UID less than 500)
- any special environment variables to be defined, are to be added to `%environment` and `%appenv` sections of recipe
- ensure the container files `/etc/passwd`, `/etc/group` and other sensitive files have nothing but the bare essentials

Things Learnt Updated

- Singularity assumes that users have access to
  - a build system where user can become root and
  - a production system where user cannot escalate privileges.
- Singularity workflow
  - develop container on own desktop (using `sudo`)
  - remote copy container to an HPC resource
  - run on the HPC resource as normal user (without `sudo` access)
- Singularity is good friends with Docker
  - no need for Docker to be installed
  - Docker images can be run/built as Singularity images
  - Docker images can be pulled
  - Docker bases and layers can be assembled into Singularity images

High Performance Computing

The selling line: Singularity was designed to run containers on HPC resources.

Essential HPC features

- **parallel execution** (multi-threaded and/or distributed)
- **accelerators** (GPUs)
- **fast disk I/O** (large data)

Desirable HPC features

- good integration with resource managers

We are discussing MPI and GPUs.

Message Passing Interface

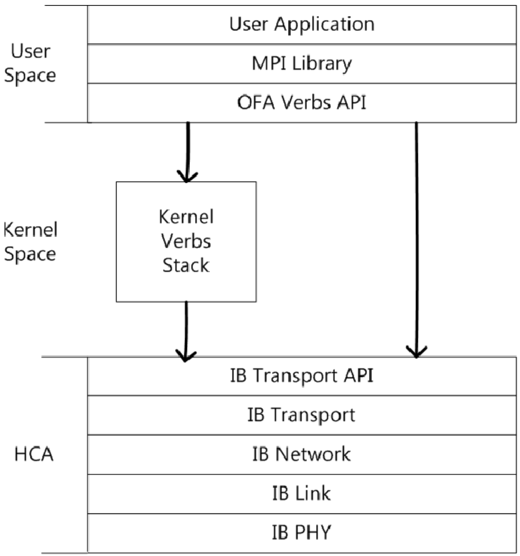
```c
#include <mpi.h>
#include <stdio.h>

int main(int argc, char ** argv){
  int size, rank;

  MPI_Init (&argc, &argv);
  MPI_Comm_size (MPI_COMM_WORLD, &size);
  MPI_Comm_rank (MPI_COMM_WORLD, &rank);

  printf ("hello from process %d of %d\n", rank, size);

  MPI_Finalize ();
}
```

```
$ mpicc hello.c -o hello
$ mpirun -np 4 ./hello
hello from process 2 of 4
hello from process 1 of 4
hello from process 3 of 4
hello from process 0 of 4
```

The MPI Standard for Distributed Computing

- syntax and semantics of a core of library routines designed for writing portable message-passing programs (in C and Fortran)
- independent processes running concurrently
  - each process executes one single program
  - each process has its own memory address space
  - processes communicate messages (data) where needed
- ensures functionality and portability
  - MPI applications compile and run without modifications

MPI Performance = Implementation + Hardware



MPI and Singularity

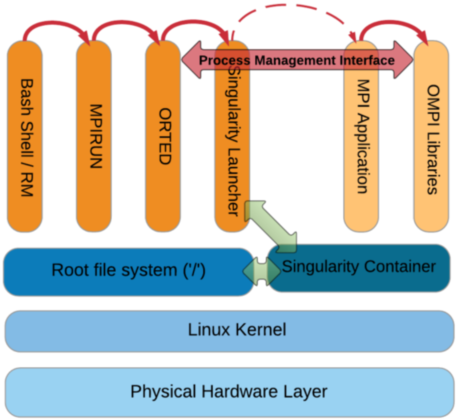
MPI components are present both inside and outside the container

- host
  - executes the `mpirun` launcher
  - controls the MPI host list
  - controls the messaging over the network
- container
  - containerised MPI libraries
  - appropriate support for Infiniband/OmniPath network

But

- OFED libraries must be containerised
- MPI software outside must be newer or equal to the container version

Out-of-the-Box Compatibility with OpenMPI



- `mpirun` called by resource manager (or directly from shell)
- OpenMPI calls the process management daemon (ORTED)
- ORTED launches container requested by `mpirun`
- Singularity builds container and namespace environment
- Singularity launches the MPI application within the container
- MPI application launches and loads the OpenMPI libraries
- OpenMPI libraries connect back to ORTED via the Process Management Interface (PMI)
- application processes run within container as they would on host

Basic Container with MPI Support

Exercise

Edit file `ubuntu-mpi-hello.def` and understand the recipe.

The recipe

- builds the OpenMPI library and
- uses the OpenMPI compiler wrappers to build two simple applications

Build the image

```
sudo singularity build ubuntu-mpi-hello.simg ubuntu-mpi-hello.def
```

Basic Container with MPI Support

```
$ mpirun -np 4 singularity exec ubuntu-mpi-hello.simg hello
hello from process 0 of 4
hello from process 1 of 4
hello from process 2 of 4
hello from process 3 of 4

$ mpirun -np 4 singularity exec ubuntu-mpi-hello.simg ring 1000

 ----- before communication
 process 0: mean of data sent to 1 = 4.865778e-01
 process 1: mean of data sent to 2 = 5.122776e-01
 process 2: mean of data sent to 3 = 5.041534e-01
 process 3: mean of data sent to 0 = 4.846409e-01

 ----- after communication
 process 0: mean of data received = 4.846409e-01
 process 1: mean of data received = 4.865778e-01
 process 2: mean of data received = 5.122776e-01
 process 3: mean of data received = 5.041534e-01

 correct communication
 communication time = 4.019204e-05
```

Singularity for MPI Applications

Exercise

Edit file `ubuntu-osu-benchmarks.def` and examine

- building the OpenMPI library is built and
- using the OpenMPI compiler wrappers to build the OSU micro-benchmarks

OSU bandwidth test (native)

```
$ mpirun -np 2 osu_bw
# OSU MPI Bandwidth Test v5.4.0
# Size      Bandwidth (MB/s)
...
4096                    3050.72
8192                    4701.28
16384                   4925.92
32768                   5414.88
65536                   5491.43
131072                  5502.49
262144                  5537.50
524288                  5577.15
1048576                 5669.64
2097152                 5576.75
4194304                 5704.30
```

OSU bandwidth test (Singularity)

```
$ mpirun -np 2 singularity exec ubuntu-osu-benchmarks.simg osu_bw
libibverbs: Warning: couldn't open config directory '/etc/libibverbs.d'.
...
[[32751,1],1]: A high-performance Open MPI point-to-point messaging module
was unable to find any relevant network interfaces:
...
Another transport will be used instead, although this may result in
lower performance.
...
--------------------------------------------------------------------------
# OSU MPI Bandwidth Test v5.4.1
# Size      Bandwidth (MB/s)
...
4096                     552.35
8192                     804.75
16384                   1006.86
32768                   1087.11
65536                    121.40
131072                   134.64
262144                   135.48
524288                   135.75
```

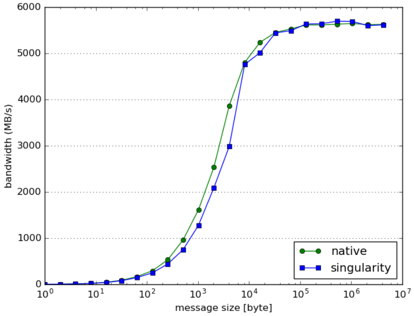
Singularity for MPI Applications

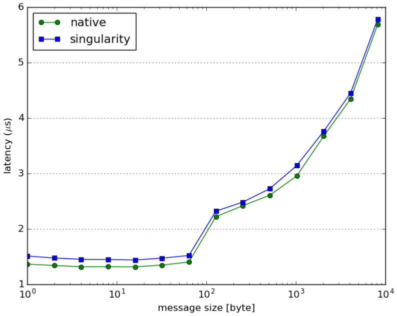
Exercise

Edit file `ubuntu-osu-benchmarks-ibverbs.def` and remark that the same recipe for building OpenMPI and the benchmarks as in `ubuntu-osu-benchmarks.def` are preceded by

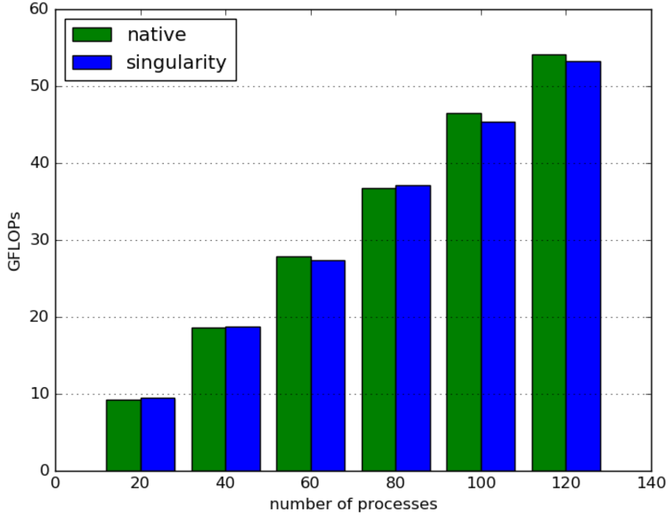
- the installation of library for InfiniBand support and
- the addition of the appropriate Linux kernel modules

OSU Benchmarks





HPCG Benchmarks



Singularity for MPI Applications

General recipe

- container library support for InfiniBand
- host OS Infiniband support and InfiniBand hardware
- covers 90% of what most users need

Improved recipe

- fine tuning by vendor specific network support in container
- example: *https://community.mellanox.com/docs/DOC-3148*
    - MLNX_OFED (Mellanox optimised OFED distribution)
    - HPC-X Toolkit (drivers, optimised engines for hardware offload, ...)

Singularity and CUDA

GPU usage
Device nodes are passed through into container Cuda libraries must be aligned with kernel drivers (similar to OFED) Workarounds exists! .The host installs Cuda/Nvidia libraries to a directory .That directory is configured as a "bind point" within-bindthe global Singularity config .The library path is added to all container's environments

- Before version 2.3, GPUs could be used only if the CUDA toolkit and NVIDIA drivers were installed in the container (problem: different versions of OS-es, compilers etc.)
- Now native support for GPUs, using –nv option, only CUDA has to be installed in the container
- This allows portability of the same container (we tested the same one on 2 different grid clusters and in Azure) and it worked

Singularity and Resource Managers

One of the architecturally defined features in Singularity is that it can execute containers like they are native programs or scripts on a host computer. As a result, integration with schedulers is simple and runs exactly as you would expect. All standard input, output, error, pipes, IPC, and other communication pathways that locally running programs employ are synchronized with the applications running locally within the container.

Things Learnt

As mentioned, user's contexts are strictly maintained and enforced This means we can safely blur the line between container and host Host/node resources can be just as tangible from within the container as outside This includes devices, file systems and paths, networks, X11, etc. This allows containers to run appropriately on HPC resources!

Thank you!