

Practical Singularity

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Dec. 2, 2020



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What is Singularity?



Singularity:

- is container software originally created by Berkeley Lab, now developed by **Sylabs.io**,
- is a **secure way** to use **Linux containers** on Linux **multi-user clusters**,
- as a way to **enable** users to have **full control of their environment**, and,
- as a way to **package scientific software** and **deploy that package** to **different clusters** having the same architecture.

URL: <https://sylabs.io>

What is Singularity?



Singularity provides **operating-system-level virtualization** called **containers**.

A **container** is not a **virtual machine**:

- containers have **very little overhead**, and,
- can only use the **same operating system** the computer uses inside the container.

What is Singularity?



Said differently:

- virtual machines, VMs, provide a virtualized interface to real hardware
 - This allows other operating systems **compatible with the computer's real hardware** to be run inside the VM.
- containers provide a virtualized interface to the operating system's kernel
 - This allows different variations of the **same** operating system to be used inside the container.

What is Singularity?



Singularity was designed to enable containers to be used securely on multi-user HPC systems without requiring any special permissions.

- Singularity is the only container technology currently supported on Compute Canada systems.

Docker is another popular container technology that is commonly used.

- Docker has a significant possible security issues making it not ideal for use on Compute Canada's clusters.
- Singularity can build images from Docker images. :-)

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Singularity is **already** installed on Compute Canada systems.

You can **install** Singularity on your own computer provided it is running **Linux** (natively or in a virtual machine).

- Installation instructions are available in the Singularity **User Guide's Quick Start** and **Administration Guide's Installation** documents.
 - e.g., https://sylabs.io/guides/3.7/user-guide/quick_start.html
 - e.g., <https://sylabs.io/guides/3.7/admin-guide/installation.html>

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To enable the use of Singularity on Compute Canada systems:

- e.g., module load singularity

If using MPI from inside a container...

- Be sure to load MPI version 3 or higher.
 - e.g., `module load openmpi/3.1.4`
 - e.g., `module load openmpi/4.0.5`
- When submitting your Slurm job script use `srun` —not `mpirun` or `mpiexec`— to run your command.
 - e.g., `srun singularity run image.sif /path/to/your-mpi-program`
- Ensure **all executables** being **run inside** the container were properly built **inside** the singularity container.

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To use Singularity you need to have or create an **image**.

- An image is a filesystem directory tree containing everything needed to run the programs inside your container.
- Not needed are the operating system kernel and boot loader software.
- Since Compute Canada runs Linux on its clusters, your Singularity container must run a variation of Linux.

Creating an image from scratch can be a lot of work. Singularity allows you to:

- build an image from **Docker Hub**, **Singularity Hub**, or a **Library**
 - Docker Hub: <https://hub.docker.com/>
 - Singularity Hub: <https://singularity-hub.org/>
 - Library defaults to <https://cloud.sylabs.io/library>
- use a container image file you already have access to,
 - *.sif Singularity Image Format (SIF); (Version v3.0 +)
 - *.sqsh SquashFS format. (Version 2.4 +)
 - *.img ext3 format. (Oldest format)
- build/run an image from a **directory**,
 - e.g., a LXC rootfs directory, a directory of your own creation
- build an image using a **Singularity recipe file**.

Some examples:

- **CentOS v7:** `singularity build centos7.sif docker://centos:7`
- **CentOS v8:** `singularity build centos8.sif docker://centos:8`
- **CentOS (latest):** `singularity build centos-latest.sif docker://centos:latest`
- **Debian v9:** `singularity build debian9.sif docker://debian:9`
- **Debian v10:** `singularity build debian10.sif docker://debian:10`
- **Debian (latest):** `singularity build debian-latest.sif docker://debian:latest`
- **Ubuntu (latest):** `singularity build ubuntu-latest.sif docker://ubuntu:latest`
- **Sandbox Directory:** `singularity build -s debian10-dir docker://debian:10`
- etc.

Images (con't)

To build from a Dockerfile, run on your own Linux computer in the same directory as the Dockerfile:

- `docker build --rm -t the-name-you-want .`
- `docker save -o the-name-you-want.tar the-name-you-want`
 - This will save the Docker image to a tarball file.

If singularity is not installed on your own computer:

- Upload `the-name-you-want.tar` to a Compute Canada cluster.
- In a shell on that cluster run `module load singularity`

Convert the Docker tarball to a Singularity container:

- `singularity build the-name-you-want.sif docker-archive://the-name-you-want.tar`
 - NOTE: You can prefix this with `sudo` if you are on your own computer and have access to root.

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There are a number of ways to use Singularity:

1. Run a **single command** which executes and then stops running.
2. Run **many commands** in an interactive session.
3. Run a container instance to run **daemons** and have **backgrounded processes**.
 - No hung processes: everything is killed when the Singularity instance is stopped/killed!

Running Commands

Given a container `image.sif` with `gcc` installed in it, one can check the version of `gcc` used with the **run** command:

```
singularity run -c image.sif gcc -v
```

Running Commands (con't)

One can interactively use the container with the **shell** command:

```
singularity shell -c image.sif
```

To exit the container type **exit**.

Running Commands (con't)

If one needs to run backgrounded and daemon processes and other commands inside the **same** running container, use the **instance start** and **instance stop** commands.

Running **instance start** with a name, e.g., `myjob`, will cause Singularity to start a new container instance:

```
singularity instance start image.sif myjob
```

Running Commands (con't)

Programs can be run using **run** or **shell** as before, except the name of the instance must be provided prefixed with **instance://**, e.g.,

```
singularity instance start image.sif myjob
singularity run -c image.sif instance://myjob ps -eaf
singularity shell -c image.sif instance://myjob
  nohup find / -type d >dump.txt
  exit
singularity run -c image.sif instance://myjob ps -eaf
```

An instance is **shut down** by running the **instance stop** command, e.g.,

```
singularity instance stop image.sif myjob
```

Bind Mounts

Programs running inside a Singularity container **will not have access to files and directories** outside of your home and the current directory (when singularity was run).

On Compute Canada to access files and directories under:

- /home
- /project
- /scratch
- /localscratch except on niagara

use the **-B, bind mount**, option when running singularity:

```
singularity shell -c -B /home -B /project -B /scratch -B /localscratch image.sif
singularity run -c -B /home -B /project -B /scratch -B /localscratch \
  image.sif gcc /project/$USER/p.c
```


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Demonstration and questions.