Containers

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Containers Overview

Shipping containers have frequently been used as an analogy for computing containers because the container is standard, it does not care what is put inside, and it will be carried on any ship; or in the case of computing containers it can run on many systems different from the one it was created on.

Docker is widely used by researchers for reasons we won’t get into here. See their documentation. Docker images cannot be run in a HPC environment. This has to do with the privileges required to run a Docker container. This issue is addressed with Singularity. It is a container technology that completely contains the authority so that all privileges needed at runtime stay inside the container. This makes it ideal for the shared environment of a supercomputer. And even better is that a Docker image can be encapsulated inside a Singularity image. So the documentation here instructs how to take either a Docker image and run it from Singularity, or create an image using Singularity only.

Singularity Overview

Singularity enables users to have full control of their environment. Singularity containers can be used to package entire scientific workflows, software and libraries, and even data. This means that you don’t have to ask your cluster admin to install anything for you - you can put it in a Singularity container and run. Did you already invest in Docker? The Singularity software can import your Docker images without having Docker installed or being a superuser. Need to share your code? Put it in a Singularity container and your collaborator won’t have to go through the pain of installing missing dependencies. Do you need to run a different operating system entirely? You can ‘swap out’ the operating system on your host for a different one within a Singularity container. As the user, you are in control of the extent to which your container interacts with its host. There can be seamless integration, or little to no communication at all. They have extensive documentation at their website.

Here are some of the use cases we support using Singularity:

• You already use Docker and want to run your jobs on HPC
• You want to preserve your environment so that a system change will not affect your work
• You need newer or different libraries than are offered on HPC systems
Someone else developed the workflow using a different version of Linux.
You prefer to use a Linux distribution other than CentOS, perhaps Ubuntu.
You want a container with a database server like MariaDB.

**Singularity Commands**

On Puma, Singularity is installed in the operating system, so the commands will work without any extra effort.

On Ocelote and ElGato, you will first need to `module load singularity`

```bash
$ singularity --help

Linux container platform optimized for High Performance Computing (HPC)

Usage:
singularity [global options...]

Description:
Singularity containers provide an application virtualization layer enabling
of compute via both application and environment portability. With one is
capable of building a root file system that runs on any Linux system where
Singularity is installed.

Options:
-d, --debug          print debugging information (highest verbosity)
-h, --help           help for singularity
-q, --quiet          suppress normal output
-s, --silent         only print errors
-t, --tokenfile string path to the file holding your sylabs
                     authentication token (default
                     "/home/u13/chrisreidy/.singularity/sylabs-token")
-v, --verbose        print additional information
--version            version for singularity

Available Commands:
build        Build a new Singularity container
capability   Manage Linux capabilities on containers
extec         Execute a command within container
help          Help about any command
inspect      Display metadata for container if available
instance     Manage containers running in the background
keys         Manage OpenPGP key stores
pull          Pull a container from a URI
push          Push a container to a Library URI
run           Launch a runscript within container
run-help      Display help for container if available
search       Search the library
shell         Run a Bourne shell within container
sign          Attach cryptographic signatures to container
test          Run defined tests for this particular container
verify        Verify cryptographic signatures on container
version       Show application version

Examples:

$ singularity help <command>

Additional help for any Singularity subcommand can be seen by appending
the subcommand name to the above command.

**Singularity Changes in Version 3.x**
For existing users two of the biggest changes are; that the file type of images now is ".sif" for Singularity Image Format for cryptographically signed and verifiable container images; and that your container may not run outside your home directory unless you include binding to other directories like /xdisk.

Singularity Hub

Singularity Hub lets you build and keep containers at their Hub. You maintain your recipes there and each time you need to pull one, it gets built there and then you retrieve the container.

This is very convenient for the scenario where you do not have access to root authority to build the container. The build takes place through the Hub.

This also lets you share containers

Singularity Remote Builder (root access)

An earlier limitation of Singularity was the requirement for access to a root account to build a container. You will not have root access on a HPC cluster. Singularity 3.0 introduced the ability to build a container in the cloud negating the root restriction.

https://cloud.sylabs.io/builder

Here is an example:

1. Log into https://cloud.sylabs.io
2. Generate an access token (API key)
3. From your working directory: module load singularity
4. singularity remote login and paste in the API key
5. singularity build --remote ~/nersc.sif nersc.recipe
6. This will produce INFO: Build complete: /home/u13/netid/nersc.sif where
7. nersc.recipe is

BootStrap: docker
From: nersc/ubuntu-mpi:14.04

%runscript
echo "This is what happens when you run the container..."

Singularity Tutorials, Examples, and Applications

- The Sylabs GitHub site has files and instructions for creating sample containers.
- We have Singularity tutorials on our Singularity Tutorials page.
- Our GitHub repository has Singularity examples available that can be run on HPC.
- There are example builds of Singularity containers for python and machine learning on our Singularity Python Methods page.

Singularity, Nvidia and GPU’s

One of the most significant use cases for Singularity is to support machine learning workflows. The details are in the GPU section. You can register at their NGC GPU Cloud site and pull your own containers. You can do this from HPC. Follow these instructions: Singularity Tutorials#PullingContainersfromNvidia