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 can run on many systems different from the one it was created on. Hence the logo for Docker, the most common container platform.

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 when the image is run all privileges 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 containers let users run applications in a Linux environment of their choosing. This is similar to but not the same as Docker.

The most important thing to know is that you create the singularity container called an image on a workstation where you have root privileges, and then transfer the image to HPC where you can execute the image. If root authority is an issue then the answer might be a virtual environment on your laptop, like Vagrant for MacOS

For an overview and more detailed information refer to:
http://singularity.lbl.gov

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 something other than Red Hat / CentOS, like Ubuntu

Singularity Commands

$ singularity --help
USAGE: singularity [global options...] <command> [command options...] ...

GLOBAL OPTIONS:
  -d|--debug    Print debugging information
  -h|--help     Display usage summary
  -s|--silent   Only print errors
  -q|--quiet    Suppress all normal output
                --version  Show application version
  -v|--verbose  Increase verbosity +1
  -x|--sh-debug Print shell wrapper debugging information

GENERAL COMMANDS:
  help       Show additional help for a command or container
  selftest   Run some self tests for singularity install

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

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 a container's metadata
  mount      Mount a Singularity container image
  pull       Pull a Singularity/Docker container to $PWD

COMMAND GROUPS:
  image     Container image command group
  instance  Persistent instance command group

CONTAINER USAGE OPTIONS:
  see singularity help <command>

For any additional help or support visit the Singularity
website: http://singularity.lbl.gov/

Singularity Tutorials

There are tutorials located here

Singularity 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.

Singularity Python and Machine Learning

More tutorials