

## Apptainer (Singularity) containers

last update: Jan 28, 2025

### Introduction

**Apptainer** (Singularity) is one of the container virtualization programs and thus have many common features with the other ones. However, there are some important differences between singularity and others (such as **Docker**), since Apptainer is explicitly focused on HPC systems. For example, non-root users can use containers without complicated prerequisites and GPUs can be used easily in Apptainer.

Contents of this page will be added from time to time.

### Container Image

Apptainer can also use Docker image (NOT ALWAYS, though). Docker images on **NVIDIA NGC** are available for example. Here is an example to build an image for apptainer (singularity) from docker one.

```
$ apptainer pull docker://nvcr.io/nvidia/pytorch:23.11-py3
```

Other References:

- Docker Hub: <https://hub.docker.com/>
- NVIDIA NGC: <https://catalog.ngc.nvidia.com/containers>

### Building Container Image

You can build Apptainer image on ccfep from the definition file. An example definition is shown below (referred to as ubuntu24\_04.def). The base environment of this container is Ubuntu 24.04. Miniforge will be installed in /opt and some of packages will be added in base environment of it. The conda environment will be loaded when loading container (%environment).

```
Bootstrap: docker
From: ubuntu:24.04

%post
apt-get -y update
apt-get -y upgrade
apt-get -y install \
  build-essential \
  wget \
  bzip2 \
  git
apt-get -y clean
wget -c https://github.com/conda-forge/miniforge/releases/latest/download/Miniforge3-Linux-x86_64.sh
/bin/sh Miniforge3-Linux-x86_64.sh -bfp /opt/miniforge
/opt/miniforge/bin/conda shell.bash hook > /opt/miniforge/conda_init.sh
. /opt/miniforge/conda_init.sh
conda install opencv numpy scipy scikit-learn jax
conda install pytest pandas sphinx curl glib glob2 isort pango
conda install path pathlib2 pathtools psutil cmake
conda install jupyterlab eigen boost transformers boost-cpp
conda install h5py markdown matplotlib
conda install scikit-image sqlite jupyter
# show list to review
conda list

%environment
. /opt/miniforge/conda_init.sh

%labels
Author RCCS
Version 0.0.1

%help
```

```
Sample python environment for RCCS supercomputer system.
```

```
%runscript
```

You can create the apptainer image (.sif) with the following command (--fakeroot option is automatically added).

```
$ apptainer build ubuntu24_04.sif ubuntu24_04.def
```

You can launch shell of the container instance.

```
$ apptainer shell ubuntu24_04.sif
(base) python
Python 3.10.14 | packaged by conda-forge | (main, Mar 20 2024, 12:45:18) [GCC 12.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

Running command example.

```
$ apptainer exec ubuntu24_04.sif gcc -dumpfullversion
13.2.0
$ apptainer exec ubuntu24_04.sif head -3 /etc/os-release
PRETTY_NAME="Ubuntu Noble Numbat (development branch)"
NAME="Ubuntu"
VERSION_ID="24.04"
```

## Notes

- Similar sample files are available in `/apl/apptainer/sample-ubuntu24.04/` directory.
- For GPUs, GPU driver of the host will be used.
  - You need to add `--nv` option when loading container. (e.g. `apptainer run --nv (sif filename)`)
  - If container requires newer GPU driver than the host one, it will result in error.
  - You may need to verify the required and installed GPU driver (or CUDA) versions.
- You can run intra-node parallel MPI program easily and effectively with the MPI environment installed in the container.
  - In this case, you can simply use `mpirun` command inside the container.
- It is not easy to run inter-node parallel MPI program, since it depends on things outside the container. Still it is possible to run MPI programs.
  - `Mpirun` command would launch multiple singularity (apptainer) commands.
  - MPI environments inside and outside of the container should be the same (or compatible?).
  - It may be difficult to get good performance. (Launching multiple container instances may not be a negligible load.)
  - It is better to avoid inter-node MPI parallel runs with singularity/apptainer.
- Your home directory will be mounted automatically. You don't need to add `/home` in `--bind`.
- If you want to use applications installed under `/apl` together with container ones, you may need to add `--bind /apl:/apl` option.
  - e.g. `apptainer run --bind /apl:/apl --nv (sif filename)`
  - You may also need `/gwork` in some cases.