# How to create a sample apptainer job.

Consider the case where you need to create a working `python3` distrib with `pytorch` installed for running a script using GPU resources on ChaCha or DISCO. On those machines, we use Apptainer for the containers and this documentation describes how to create, customize and run images using Apptainer. Launching Apptainer tasks using Slurm is defined elsewhere.

## Define the content of the container

Define a container definition, such as in `rules.def` (this correponds to a `Dockerfile` file):

```
Bootstrap: docker
From: nvidia/cuda:12.6.2-base-ubuntu22.04

%help
  This container provides a CUDA environment, with Python and
Jupyternotebook.

%labels
  AUTHOR_NAME Pierre-André Mudry
  VERSION 1.0

%environment

%post -c /bin/bash
  export DEBIAN_FRONTEND=noninteractive
  apt-get -y update
  apt-get -y install git python3-pip python3-dev python3-opencv libglib2.0-0

%files
  requirements.txt requirements.txt

%post -c /bin/bash
  python3 -m pip install -r requirements.txt
  python3 -m pip install --upgrade pip
  pip3 install torch torchvision torchaudio -f
https://download.pytorch.org/whl/cu111/torch_stable.html
```

This definition files is of a Debian distrib with CUDA, with `python3` and `pytorch` installed and has other requirements as well. Those requirements are copied from you current directory `requirements.txt` file using the `%files` directive. In this example, we use for `requirements.txt`:

```
warp-lang
usd-core
matplotlib
pyglet
```

```
jupyter
python-language-server
```

Of course, you can tailor this to fit your needs.

# Building the image

Once the definition is made, you can build the `test.sif` image with `apptainer build test.sif rules.def`. The image is created in your own directory. By default, when you run the image, it has access to the host filesystem. To run the image interactively (or not), you then simply run

# Running the image

```
apptainer run --nv ./test.sif
```

The `--nv` flag must be used to use NVidia resources. If your run this script interactively, you then have access to the virtual environment. You can launch for instance `nvidia-smi` or `jupyter notebook --ip=0.0.0.0 --port=8888 --no-browser --allow-root` to create a Juypter notebook system.

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