

Building Conda environments in Apptainer

Apptainer is a containerization technology forked from Singularity. It's free, open source and compatible with Docker and Singularity images. This has the advantage of keeping all of your Conda environment programs in one convenient file and avoiding conflicts and problematic entanglements with other Conda environments on the same machine.

Apptainer containers are built from a definition file, let's start with this example below:

```
Bootstrap: docker
From: continuumio/miniconda3

%post -c /bin/bash
    # Update and install system wide software here
    apt-get update -y
    # if you need apt packages install them here
    # apt-get install <package>

    # install conda stuff here, numpy just for example
    conda install -y numpy

%environment
    # Ensure Conda environment is in the PATH
    PATH="/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin:$PATH"
    source /opt/conda/etc/profile.d/conda.sh
    conda activate base
```

Save this file to MyCondaEnv.def on a machine with Apptainer installed. HPC1 is a fine place to do this as we have Apptainer available there for building images. You can also do it on your local machine and upload the resulting SIF file to HPC1 at a later date.

Now is time to build the image:

```
apptainer build --fakeroot MyCondaEnv.sif MyCondaEnv.def
```

This may take a minute or two.

After it has successfully finished you'll be left with the MyCondaEnv.sif file. This is where the actual Conda binaries and packages are stored. Once created it cannot be modified and has to be rebuilt if you want to add a new package.

Now you can run the Apptainer image and interact with your data in one of two primary ways. Firstly through apptainer exec:

```
apptainer exec MyCondaEnv.sif conda list
```

Where everything after the SIF file will be run inside the container. This prints a list of installed conda packages. Alternatively you can use apptainer run and it will drop you into a shell on the container.

```
[lh59281@hpc2 ~]$ apptainer run MyCondaEnv.sif
(base) ls
AstroInteractives  Pictures          apptainer_test.sh          gauss_test.log
jupyter2           jupyternoRoot.def other_data                  processing         test_mpi
Desktop            Public           conda.def                  gpu_test.bsh
jupyterhub.sqlite  lh59281_lambda  output-9604.log          shiny-server.def  test_mpi.c
(base)
```

Notice that here I just did a ls and it lists my home directory. You can any program installed in the Apptainer container on data stored in your home directory.

It is recommended to submit the actual running of the computations through Slurm or use Apptainer via the [Virtual Desktops](#) available in [Open OnDemand](#).

Let's say you forgot a Conda package and need to add it. If you try to install it from inside the Apptainer shell you'll get an error:

```
EnvironmentNotWritableError: The current user does not have write permissions to the target
environment.
  environment location: /opt/conda
  uid: 1002
  gid: 1002
```

These containers are create once, read only and easily rebuilt so the solution is to exit your container shell (Ctrl+D) and make a new container. First let's update the DEF file:

```
Bootstrap: docker
From: continuumio/miniconda3

%post -c /bin/bash
```

```
# Update and install system wide software here
apt-get update -y
# if you need apt packages install them here
# apt-get install <package>

# install conda stuff here, numpy just for example
# adding astropy here for a rebuild example
conda install -y numpy astropy

%environment
# Ensure Conda environment is in the PATH
PATH="/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin:$PATH"
source /opt/conda/etc/profile.d/conda.sh
conda activate base
```

Now build a new container:

```
apptainer build --fakeroot MyCondaEnv2.sif MyCondaEnv.def
```

After that has completed, run it as before:

```
apptainer run MyCondaEnv2.sif
```

Verify the new packages are loaded:

```
[lh59281@hpc2 ~]$ apptainer run MyCondaEnv2.sif
(base) conda list | grep astropy
astropy                7.0.0                py313h5eee18b_0
astropy-iers-data      0.2025.6.23.0.39.50 py313h06a4308_0
(base)
```

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