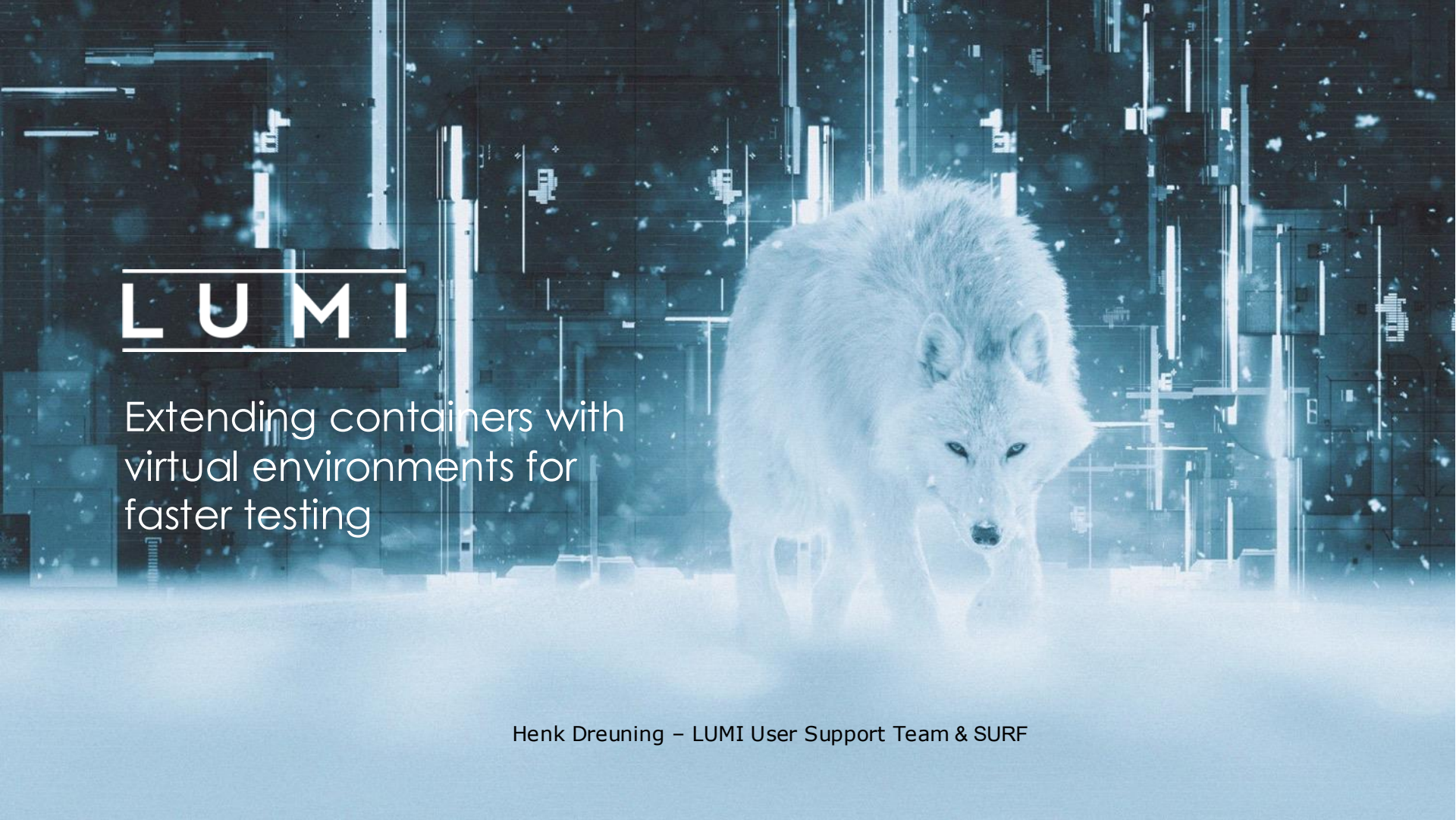

Extending containers with virtual environments for faster testing

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Motivation

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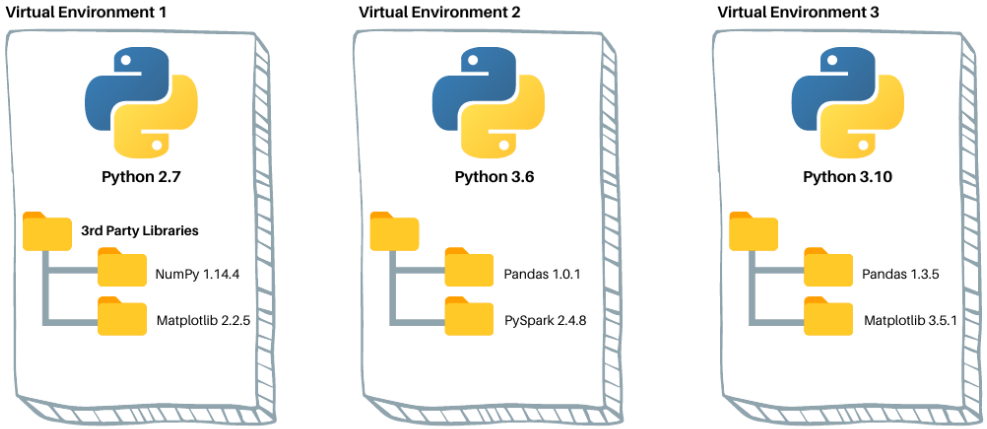
Cotainr is great, but building a container takes time --> not ideal for quick testing / iterating on your project

Virtual environments offer a quick (and easy) way of installing additional packages to existing containers

What are virtual environments

A virtual environment is a folder tree containing a specific Python version, third-party libraries, and other scripts.



Source: www.dataquest.io/blog/a-complete-guide-to-python-virtual-environments/ dataquest.io

Virtual environments are conceptually similar to `conda` environments – just for `pip` only.

Requirements

We assume we already have a container built from a conda environment file. If not, we can build one via:

```
module load LUMI/25.03 cotainr

BASE_CONTAINER=/appl/local/laifs/containers/lumi-multitorch-u24r70f21m50t210-20260513_121430/lumi-multitorch-mpich-u24r70f21m50t210-20260513_121430.sif

cotainr build minimal_pytorch.sif --base-image=$BASE_CONTAINER --conda-env=minimal_pytorch.yml --accept-license
```

```
name: minimal_pytorch
channels:
  - conda-forge
dependencies:
  - filelock=3.29.0
  - fsspec=2026.4.0
  - jinja2=3.1.6
  - markupsafe=3.0.3
  - mpmath=1.3.0
  - networkx=3.6.1
  - numpy=2.4.6
  - pillow=12.2.0
  - pip=24.0
  - python=3.12.3
  - sympy=1.14.0
  - typing-extensions=4.15.0
  - pip:
    - --extra-index-url https://download.pytorch.org/whl/rocm7.0/
    - triton-rocm==3.6.0
    - torch==2.10.0+rocm7.0
    - torchaudio==2.10.0+rocm7.0
    - torchvision==0.25.0+rocm7.0
```

Run a shell inside the container

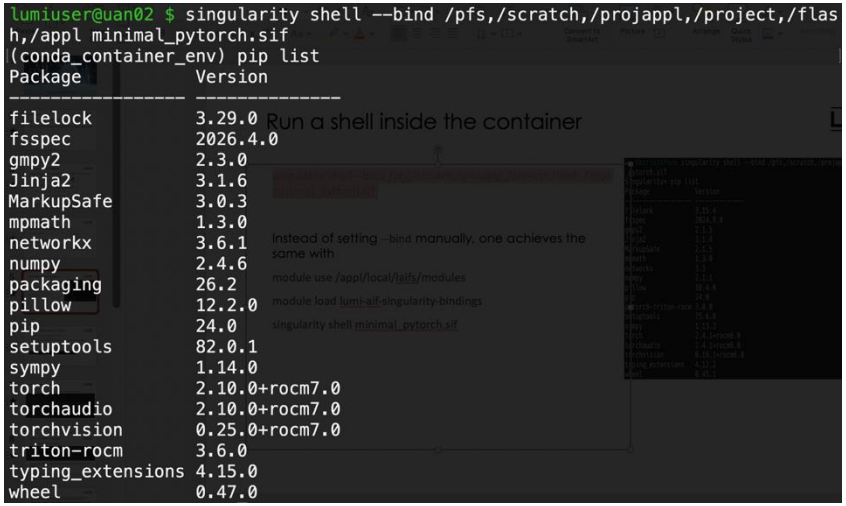
singularity shell --bind /pfs,/scratch,/projappl,/project,/flash,/appl minimal_pytorch.sif

Instead of setting --bind manually, one achieves the same with

module use /appl/local/laifs/modules

module load lumi-aif-singularity-bindings

singularity shell minimal_pytorch.sif



Create a virtual environment via venv

Inside the container, create a virtual environment via venv

```
python -m venv myenv --system-site-packages
```

The --system-site-packages flag gives the virtual environment access to the packages inside the container.

Activate the environment via

```
source myenv/bin/activate
```

```
(conda_container_env) python -m venv myenv --system-site-packages
(conda_container_env) source myenv/bin/activate
(myenv) (conda_container_env)
```

Install custom packages via pip

pip install torchmetrics

The new package will then be available alongside the packages in the container

```
(myenv) (conda_container_env) pip install torchmetrics
Collecting torchmetrics
  Downloading torchmetrics-1.9.0-py3-none-any.whl.metadata (23 kB)
Requirement already satisfied: numpy>1.20.0 in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from torchmetrics) (2.4.6)
Requirement already satisfied: packaging>17.1 in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from torchmetrics) (26.2)
Requirement already satisfied: torch>=2.0.0 in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from torchmetrics) (2.10.0+rocm7.0)
Collecting lightning-utilities>=0.15.3 (from torchmetrics)
  Downloading lightning_utilities-0.15.3-py3-none-any.whl.metadata (5.5 kB)
Requirement already satisfied: typing_extensions in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from lightning-utilities>=0.15.3->torchmetrics) (4.15.0)
Requirement already satisfied: filelock in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from torch>=2.0.0->torchmetrics) (3.29.0)
Requirement already satisfied: setuptools in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from torch>=2.0.0->torchmetrics) (82.0.1)
Requirement already satisfied: sympy>=1.13.3 in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from torch>=2.0.0->torchmetrics) (1.14.0)
Requirement already satisfied: networkx>=2.5.1 in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from torch>=2.0.0->torchmetrics) (3.6.1)
Requirement already satisfied: jinja2 in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from torch>=2.0.0->torchmetrics) (3.1.6)
Requirement already satisfied: fsspec>=0.8.5 in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from torch>=2.0.0->torchmetrics) (2026.4.0)
Requirement already satisfied: triton-rocm==3.6.0 in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from torch>=2.0.0->torchmetrics) (3.6.0)
Requirement already satisfied: mpmath<1.5,>=1.1.0 in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from sympy>=1.13.3->torch>=2.0.0->torchmetrics) (1.3.0)
Requirement already satisfied: MarkupSafe>=2.0 in /opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages (from jinja2->torch>=2.0.0->torchmetrics) (3.0.3)
Downloading torchmetrics-1.9.0-py3-none-any.whl (983 kB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 983.4/983.4 kB 2.5 MB/s eta 0:00:00
Downloading lightning_utilities-0.15.3-py3-none-any.whl (31 kB)
Installing collected packages: lightning-utilities, torchmetrics
Successfully installed lightning-utilities-0.15.3 torchmetrics-1.9.0
```

Location of installed packages

We can check the location of the installed files via

```
(myenv) (conda_container_env) python
Python 3.12.3 | packaged by conda-forge | (main, Apr 15 2024, 18:38:13) [GCC 12.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import os
>>> import torchvision
>>> import torchmetrics
>>> os.path.abspath(torchvision.__file__)
'/opt/cotainr/conda/envs/conda_container_env/lib/python3.12/site-packages/torchvision/__init__.py'
>>> os.path.abspath(torchmetrics.__file__)
'/pfs/lustrep1/projappl/project_462000008/hdreuning/AI_workshop_2026/myenv/lib/python3.12/site-packages/torchmetrics/__init__.py'
```

The new package is installed in our virtual environment whereas the other packages are installed in the container.

Warning

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You should not stop here, as this way of installing python packages creates typically thousands of small files. This puts a lot of strain on the Lustre file system and might exceed your file quota.

Once you have a complete set of python packages and their versions, choose one of the following options:

- Create a new container with `cotainr` and delete virtual environment
- Turn `myenv` into a SquashFS file and bind mount it to the container

Option 1: Create a new container with cotainr

After having found all needed packages, add them to the conda environment file and create a new container:

```
module load LUMI/25.03 cotainr

BASE_CONTAINER=/appl/local/laifs/containers/lumi-multitorch-u24r70f21m50t210-20260513_121430/lumi-multitorch-mpich-u24r70f21m50t210-20260513_121430.sif

cotainr build updated_pytorch.sif --base-image=$BASE_CONTAINER --conda-env=updated_pytorch.yml --accept-license
```

The virtual environment should then be deleted:

```
rm -rf myenv
```

```
name: minimal_pytorch
channels:
  - conda-forge
dependencies:
  - filelock=3.29.0
  - fsspec=2026.4.0
  - jinja2=3.1.6
  - markupsafe=3.0.3
  - mpmath=1.3.0
  - networkx=3.6.1
  - numpy=2.4.6
  - pillow=12.2.0
  - pip=24.0
  - python=3.12.3
  - sympy=1.14.0
  - typing-extensions=4.15.0
  - pip:
    - --extra-index-url https://download.pytorch.org/whl/rocm7.0/
    - triton-rocm==3.6.0
    - torch==2.10.0+rocm7.0
    - torchaudio==2.10.0+rocm7.0
    - torchvision==0.25.0+rocm7.0
    - torchmetrics==1.9.0
```

Option 2: Turn myenv into a SquashFS file

Turn the myenv directory into a SquashFS file:

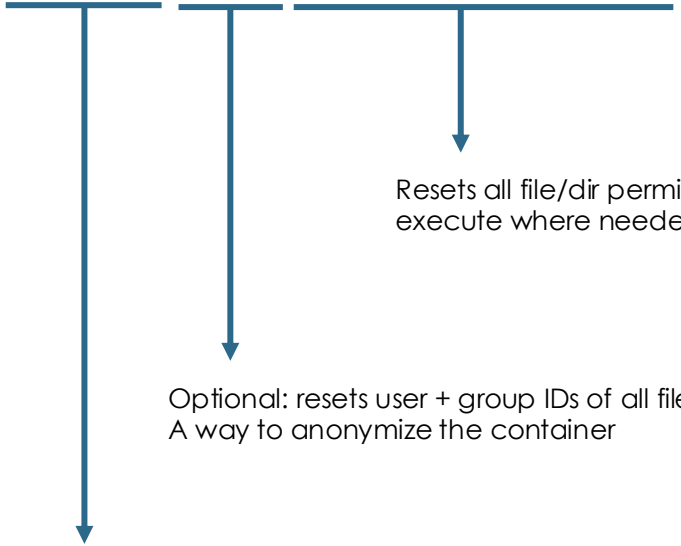
```
mksquashfs myenv myenv.sqsh
rm -rf myenv
```

Option 2: Turn myenv into a SquashFS file

Turn the myenv directory into a SquashFS file:

```
mksquashfs myenv myenv.sqsh -processors 1 -all-root -action "chmod(a+rX) @true"

rm -rf myenv
```



Resets all file/dir permissions to read (and execute where needed) for everybody

Optional: resets user + group IDs of all files to root
A way to anonymize the container

Use 1 core to keep load on login node low
Can use 1-16

Option 2: Turn myenv into a SquashFS file

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Bind mount it to the container:

```
export SINGULARITYENV_PREPEND_PATH=/user-software/bin
singularity exec -B myenv.sqsh:/user-software:image-src=/ minimal_pytorch.sif python my_script.py
```

This is much better for the file system as it regards the myenv.sqsh as a single file.

For advanced users:

This approach is compatible with packages that cannot be installed via cotainr (e.g. packages that require manual compilation)

Option 2: Adding more packages: un-squash myenv

It is also possible to un-squash the file:

```
unsquashfs -d ./myenv -processors 1 myenv.sqsh
```

Use the same steps as before to add more packages to the venv and squash it again.

Pros and Cons

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Pros:

- Quick (and easy) approach for installing additional packages to existing containers

Cons:

- Additional packages are installed directly on Lustre file system which can lead to bad performance and exceed your file limit (if `SquashFS` approach is not used)
- Necessary to source the `venv` / set `SINGULARITYENV_PREPEND_PATH` to get access to the packages in the virtual environment from inside the container
- Required to keep manually track of which `venv` matches which container for which use case

Summary of steps

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Open shell inside container

```
singularity shell --bind
/pfs,/scratch,/projappl,/project,/flash,/appl
container_image.sif
```

Create and activate a virtual environment:

```
python -m venv myenv --system-site-packages

source myenv/bin/activate
```

Install custom packages

```
pip install new_package
```

Make SquashFS file:

```
mksquashfs myenv myenv.sqsh -processors 1 -all-root
-action "chmod(a+rX) @true"
```

Remove venv:

```
rm -rf myenv
```

Bind and use SquashFS file:

```
export SINGULARITYENV_PREPEND_PATH=/user-
software/bin

singularity exec -B myenv.sqsh:/user-software:image-
src=/ container_image.sif python my_script.py
```

Un-squash to add packages after squashing:

```
unsquashfs -d ./myenv -processors 1 myenv.sqsh
```