LUMI

Building containers from conda/pip environments

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Conda environment.yml files

LUMI

- A conda environment can be described in a YAML file
- You may write this file yourself
  - Prefer conda packages over pip
  - Pin version numbers (and ideally also build numbers)
    Format: <package_name>=<version>=<build_number>
- You may export an already existing conda environment

```
conda env export -n <name_of_conda_env> -f conda_env.yml
```

- Installing the conda enviornment is easy

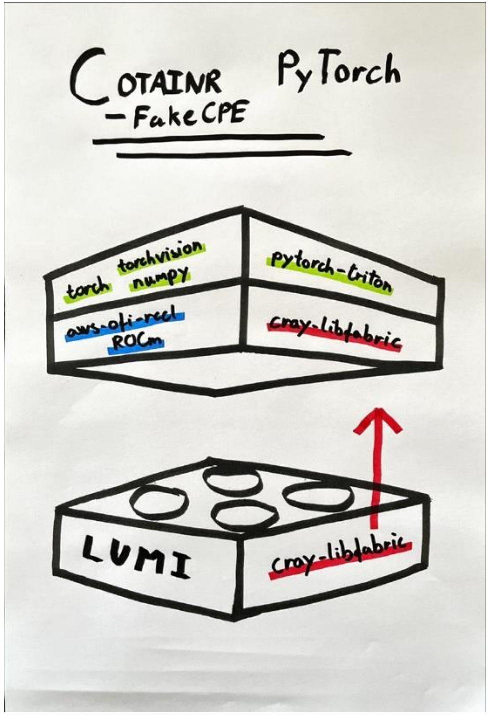
```
conda env create -f conda_env.yml
```

- We ask you to **NOT** install such conda environments directly on the Lustre files systems (/project, /scratch, /flash or your home folder) - use a container instead
  - But how do I easily build a container from a conda_env.yml file?

```
name: PandasAI
channels:
  - conda-forge
dependencies:
  - pandas=1.5.3
  - pip=24.0
  - python=3.12.3
  - ...
  - pip:
    - pandasai==2.0.35
    - ...
```

Building containers for LUMI

- Separation of concerns:
  - Host libraries (OS, drivers, container runtime, …)
    - Provided by the LUMI system administrators
  - System specific libraries (ROCm, aws-ofi-rccl, …)
    - Provided by the LUMI User Support Team as container base images
  - Application libraries (PyTorch, NumPy, …)
    - Provided by **you**
- **For application libraries specified in a conda_env.yml file, you may use *cotainr* to easily build a container on LUMI**
- For the more general case, Singularity + proot may be used to build containers on LUMI



Cotainr
– the shortcut to building containers based on conda environments

- Instead of

  ```
  conda env create -f my_AI_env.yml
  ```

  you run*

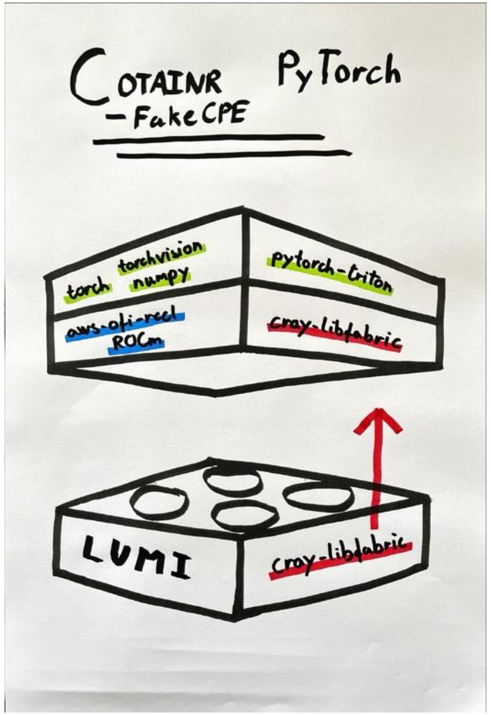
  ```
  cotainr build my_AI_container.sif --system=lumi-g
   --conda-env=my_AI_env.yml
  ```

- The `--system=lumi-g` is a shortcut to getting a proper base image. Alternatively, specify `--base-image=...`
- Cotainr is installed in the central LUMI software stack

```
module purge
module load CrayEnv cotainr
```

- To avoid putting stress on the login-nodes, you may consider running cotainr non-interactively on a compute node

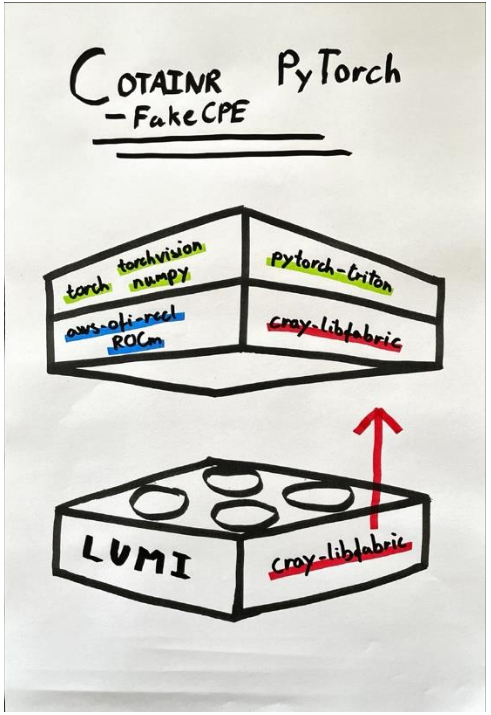
```
srun --output=cotainr.out --error=cotainr.err --account=<project_ID>
   --time=00:30:00 --mem=64G --cpus-per-task=32 --partition=debug
   cotainr build minimal_pytorch.sif --system=lumi-g --conda-
   env=minimal_pytorch.yml --accept-licenses
```



* The my_AI_env.yml Conda environment file must specify packages that are compatible with the GPUs on LUMI, i.e. ROCm builds of PyTorch/Tensorflow/Jax/...

Cotainr
– Pros & Cons

- Alternatives
  - No container – pip/conda directly on file sytem
    Problem: Many files will cause you issues with your quota and affects the file system performance
  - Self-built containers
    Not straighforward to built conda environment inside container.
    Especially difficult to get communication right
  - Prebuilt LUMI containers
    Limited packaes included → expanding can be difficult and error prone
- Pros of cotainr
  - Very easy to use
  - Forces good practises on how to use conda
- Cons of cotainr
  - Building containers takes time
  - Internode communication doesn't work at the moment on LUMI-C
  - Only works for packages that can be installed with conda/pip



A note on ROCm compatibility for LUMI-G

- To have AMD GPU support, you need ROCm compatible versions of:
  - The AMDGPU/KFD Linux kernel driver – installed by the LUMI system administrators
  - The ROCm user space components – included in the base image
  - The application built with ROCm support – the conda/pip package (or source) selected by you
- AMD only provides a +/- 2 ROCm release "tested compatibility" claim
  - As of February 2025, the AMDgpu driver on LUMI, aligned with ROCm 6.0, has "tested compatibility" with ROCm versions 5.6, 5.7, 6.0, 6.1, and 6.2.
  - The most recent ROCm release, 6.3, is not fully supported on LUMI
  - Historically, we have seen 4-5 ROCm releases a year, roughly corresponding to a "tested compatibility" window of about +/- ½ year. Thus, older versions of ROCm quickly become unsupported on LUMI following system upgrades
  - Applications are typically built for a range of ROCm releases, providing a larger compatibility window, but you might not be able to run very old or the most recent versions of PyTorch/TensorFlow/Jax/... on LUMI

A note on pip installable software

- Anything you can specify in a pip requirements.txt file, you can specify in the same way in the pip section of a conda_env.yml file.
- Thus, ANY binary/source that installs using a pip requirements.txt file can be installed using cotainr, e.g.
    - Standard PyPI packages (wheels or from source)
    - Local wheels or source archives
    - Wheels or source archives hosted on blob storage, e.g. LUMI-O
    - Git(Hub/Lab) repos that contain a proper setup.py (or the more modern pyproject.toml)
- If you need to install something from source that needs to compile C and/or ROCm extensions, you must make sure everything needed is available for pip to build and install the software, i.e. you must
    - Install all necessary libraries and compilers if they are not part of the base image, e.g. as conda dependencies in your conda_env.yml
    - Set/export any required environment variables for the build
    - Make sure that any CUDA extensions have been ported to HIP/ROCm
- Consider building wheels for source or local projects separately from building containers to maximize reproducibility.

Cotainr repices:
PyTorch for LUMI-G

- No official conda package for ROCm PyTorch exists, but official pip wheels do exist
  - Browse available versions at: https://download.pytorch.org/whl/
  - Add the --extra-index-url https://download.pytorch.org/whl/<rocm-version> to your conda environment pip specification
  - Add the relevant "+rocmX.Y" package to your conda environment pip specification
- Building the container on LUMI:
- `module load CrayEnv cotainr`

```
cotainr build minimal_pytorch.sif
    --system=lumi-g
    --conda-env=minimal_pytorch.yml
```

minimal_pytorch.yml

```
name: minimal_pytorch
channels:
  - conda-forge
dependencies:
  - filelock=3.15.4
  - fsspec=2024.9.0
  - jinja2=3.1.4
  - markupsafe=2.1.5
  - mpmath=1.3.0
  - networkx=3.3
  - numpy=2.1.1
  - pillow=10.4.0
  - pip=24.0
  - python=3.12.3
  - sympy=1.13.2
  - typing-extensions=4.12.2
  - pip:
    - --extra-index-url
https://download.pytorch.org/whl/rocm6.0/
    - pytorch-triton-rocm==3.0.0
    - torch==2.4.1+rocm6.0
    - torchaudio==2.4.1+rocm6.0
    - torchvision==0.19.1+rocm6.0
```

Further reading

- LUMI Docs containers page
  https://docs.lumi-supercomputer.eu/software/containers/singularity/
- LUMI Docs installing Python packages page
  https://docs.lumi-supercomputer.eu/software/installing/python/
- Cotainr conda env documentation
  https://cotainr.readthedocs.io/en/latest/user_guide/conda_env.html
- Conda environment documentation
  https://conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html
- Pip requirements.txt file specification
  https://pip.pypa.io/en/stable/reference/requirements-file-format/
- ROCm compatibility kernel / user space compatibility
  https://rocm.docs.amd.com/projects/install-on-linux/en/latest/reference/user-kernel-space-compat-matrix.html