Conda - Reproducible Python Environments

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Conda & Anaconda & Mamba

- **`conda`** is the package manager core.
- **`miniconda`** is the package we installed to provide conda.
- **`anaconda`** is a proprietary (unfree!) summary of packages.
- **`mamba`** was a faster sister of conda.
- **`micromamba`** sister of miniconda.

we focus on `conda` via `miniconda`.

Start Conda

First load the **miniconda** package with `module` (or `spack`):

```
zen trainee00@l55:~$ module load miniconda3
```

Start **conda bash hook** to get the conda functions:

```
zen trainee00@l55:~$ eval "$(conda shell.bash hook)"
(base) zen trainee00@l55:~$ conda
usage: conda [-h] [-v] [--no-plugins] [-V] COMMAND ...

conda is a tool for managing and deploying applications,
environments and packages.

...
```

Note how the prompt now shows the **base** env.

Define Your Environment

Create a `yaml` file **defining** your environment.

```yaml
name: myenv
channels:
  - conda-forge
  - defaults
dependencies:
  - python=3.10
  - tensorflow=2.15.0
```

Use e.g. `nano myenv.yaml` to write this file.

Create Your Environment

Create your conda env:

```
(base) zen trainee00@l55:~$ conda env create --file myenv.yaml
Channels:
 - conda-forge
 - defaults
 - bioconda
Platform: linux-64
Collecting package metadata (repodata.json): /
...
```

Depending of the number of packages this might take some time.

Activate Your Environment

Activate your conda env, note how the **prompt** changes:

```
(base) zen trainee00@l55:~$ conda env create --file myenv.yaml
(base) zen trainee00@l55:~$ conda activate myenv
...
(myenv) zen trainee00@l55:~$ python --version
Python 3.10.11
```

The python version shown is the installation from conda.

Submit Your Conda Env To Slurm

Create a slurm batch script starting your conda env and running python:

```bash
#!/bin/bash
#SBATCH --job-name=slurm_conda_example
#SBATCH --time=00-00:05:00
#SBATCH --ntasks=2
#SBATCH --mem=2GB

module load miniconda3
eval "$(conda shell.bash hook)"
conda activate myenv
python --version
```

Use e.g. `nano myenv.sh` to write this file.

List All Environments

```
(base) zen trainee00@l55:~$ conda env list
# conda environments:
#
myenv        /home/fs70824/trainee00/.conda/envs/myenv
base      *  /opt/sw/conda
py310        /opt/sw/conda/envs/py310
py311        /opt/sw/conda/envs/py311
py312        /opt/sw/conda/envs/py312
py38         /opt/sw/conda/envs/py38
py39         /opt/sw/conda/envs/py39
```

The star * shows the currently active environment.

Deactivate Your Environment

Deactivate your conda environment to get back to `(base)`:

```
(myenv) zen trainee00@l55:~$ conda deactivate
(base) zen trainee00@l55:~$ conda deactivate
zen trainee00@l55:~$
```

Type `conda deactivate` again to **get out** of conda completely.

Remove Your Environment

If you don't need them anymore please **remove** any old environments:

```
(base) zen trainee00@l55:~$ conda env remove -n myenv

Remove all packages in environment /home/fs70824/trainee00/.conda/env
s/myenv:

Everything found within the environment (/home/fs70824/trainee00/.con
da/envs/myenv), including any conda environment configurations and an
y non-conda files, will be deleted. Do you wish to continue?
 (y/[n])?
```

Conda creates **many small files** and might fill up your `$HOME` file system quickly.

▶ make a new empty directory `contest` to play around in.
▶ load **miniconda3**.
▶ write your own `conda.yaml` and install **numpy**.
▶ create a new env based on your `conda.yaml`.
▶ activate your env.
▶ find out what version of python is running there.
▶ submit a job to `slurm` printing the python version.
▶ deactivate and remove your environment.

Links

▶ There is a lot about python, conda and jypyter at our **python4hpc** courses:

https://vsc.ac.at//research/vsc-research-center/vsc-school-seminar/

▶ In depth `jupyter` notebooks (`ipynb`) from the python4hpc course:

https://gitlab.tuwien.ac.at/vsc-public/training/python4hpc/-
/blob/main/D1_02_env_03_conda.ipynb

▶ Some basic usage like this example on our wiki:

https://wiki.vsc.ac.at/doku.php?id=doku:python