Software distribution with Conda

Conda package manager

Conda is a cross-platform, language-agnostic binary package manager

- Open Source and main developer is Continuum Analytics
- Anaconda Python distribution
- Miniconda minimal Python distribution
- conda build for building packages
- Anaconda Cloud for hosting packages
- Possibiliby to host your own packages and channels

Channels

Conda channels are the locations where packages are stored

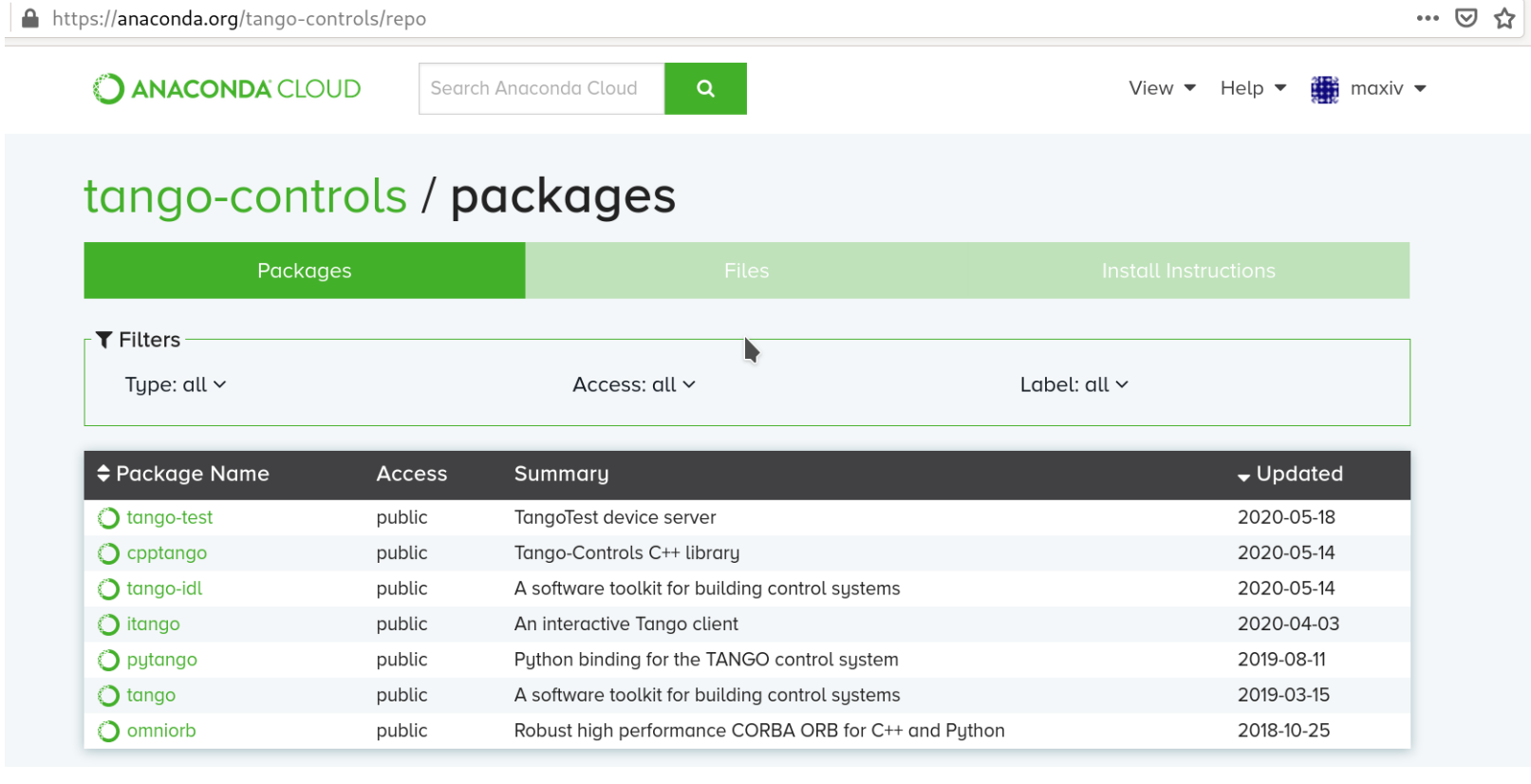
- **Defaults**: Maintained by Continuum Analytics
  Provides optimized BLAS support in numpy (Intel MKL)
  Tensorflow with Cuda support tensorflow-gpu
- **Conda-forge**: Maintained by the open source community
  More packages than in the defaults channel
  Updated more frequently

Order of channels matter for resolving dependencies

```
conda config --add channels conda-forge
conda config --append channels conda-forge
```

Custom Channels

Ability to create custom channels for software that is not available in other channels



Building own packages with conda-build

```
conda-build mypackage
```

```
{% set version = "9.3.2" %}

package:
  name: pytango
  version: {{ version }}

source:
  url: https://github.com/tango-controls/pytango/archive/v{{ version }}.tar.gz
  patches: libtango.patch

build:
  number: 5
requirements:
  build:
    - {{ compiler('cxx') }}
  host:
    - cpptango
    - python
    - boost
    - numpy
    - cppzmq
  run:
    - python
    - cpptango
    - {{ pin_compatible('boost', max_pin='x.x') }}
    - numpy
```

Conda environments

A conda environment is a directory that contains a specific collection of conda packages that you have installed

Create new environment

```
conda create -n myenv python=3.8 numpy h5py scipy
```

Activate environment

```
conda activate myenv
```

Install package in current environment

```
conda install matplotlib
```

List packages in current environment

```
conda list
```

Conda at MAX IV

Compute cluster

```
module load Anaconda3/2020.02
```

Shared Conda on NFS

/mxn/groups/pub/sw/pkg/anaconda3

```
source /mxn/groups/pub/sw/source_me_for_anaconda
```

User environments will be installed in Home directory by default (they can get quite large, be careful with disk quota)

In [1]:
```
conda info
```

```
     active environment : analysis
    active env location : /home/clemens/miniconda3/envs/analysis
            shell level : 2
       user config file : /home/clemens/.condarc
 populated config files : /home/clemens/.condarc
          conda version : 4.8.3
    conda-build version : 3.18.11
         python version : 3.8.2.final.0
       virtual packages : __glibc=2.31
       base environment : /home/clemens/miniconda3  (writable)
           channel URLs : https://conda.anaconda.org/maxiv/linux-64
                          https://conda.anaconda.org/maxiv/noarch
                          https://conda.anaconda.org/conda-forge/linux-64
                          https://conda.anaconda.org/conda-forge/noarch
                          https://repo.anaconda.com/pkgs/main/linux-64
                          https://repo.anaconda.com/pkgs/main/noarch
                          https://repo.anaconda.com/pkgs/r/linux-64
                          https://repo.anaconda.com/pkgs/r/noarch
          package cache : /home/clemens/miniconda3/pkgs
                          /home/clemens/.conda/pkgs
       envs directories : /home/clemens/miniconda3/envs
                          /home/clemens/.conda/envs
               platform : linux-64
             user-agent : conda/4.8.3 requests/2.23.0 CPython/3.8.2 Linux/5.6.
15-arch1-1 arch/ glibc/2.31
                UID:GID : 1000:1000
             netrc file : None
           offline mode : False


Note: you may need to restart the kernel to use updated packages.
```