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Ana/Mini/Conda

or "How to completely wipe and reinstall your complete scientific Python stack in under 5 minutes" (if you have to)

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Scripts at this gist

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Conda vs Anaconda vs Miniconda

- Questions to audience:
- How many here use any conda-based system?
- How many understand the differences between the different conda terms in the title of this slide?
- Before we expunge/reinstall, let's understand it better.

Conda vs Anaconda vs Miniconda (2)



Standard conda package (grey)

Conda also manages virtual envs

 If you only ever need one environment, you could stay with graphical Conda installer, however...

conda create -n py37 python=3.7 spiceypy matplotlib numpy



Legacy Python:

conda create -n py2 python=2 python2_package

Use "**conda activate <env-name>**" to switch between environments.

My python package search tree

- First conda: conda install <pkg_name>
 - The dependency resolver will tell if it would lead to downgrades of other packages, you can inspect and reject at this point.
- What if a Python package is not available conda?
 - pip install pkg_name
 - NOTE: Always do conda activate <env_name> before this (or anything really). Because otherwise a different "pip" command might be used on your computer and install goes somewhere else.
 - Pip ALWAYS depends on current active conda environment (or PATH if no conda)
 - If you ever did "pip install" and then Python couldn't find it, it didn't install where you think it did.
- What if pkg not even on Pypi server? Find it on GitHub:
 - git clone <url_copied_from_GitHub && cd <cloned_repo> && pip install (-e) .
- I use this mix for many years successfully.

Conda vs Anaconda vs Miniconda (3)

- So, in summary:
 - conda is the **executable** that manages packages (not only Python, e.g. HDF binaries, FORTRAN, OpenCV, GDAL libraries etc.)
 - "miniconda" is a minimum set of packages for proper operation of conda, installed into a "base". Use this if you understand conda well.
 - "anaconda" is a meta-package with a huge list of scientific packages (dependencies) (**Recommended for beginners**)
 - Hence: after installing miniconda and executing "conda install anaconda", you would have the same python env as somebody that DL-ed the Anaconda distribution.

Everyday conda (terminal) tips

- If you have installed it before, and it's older than conda 4.6, remove and reinstall everything.
 - New version (now at 4.8.x) is much faster in adding a new package
 - Too many changes that make it better to delete "old cruft"
- If you still have changed PATH changes that point to your conda install in your ba/c/tc-sh configs, remove it!
 - Call of "conda init <shell_name>" configures things correctly, adding an init section to config files.
 - Leaving the manual PATH change in can create problems.
- Advise: Don't use the initial conda "base" environment for general work.
 - Eventually some of your installs (or Anaconda, Inc.) will mess up something.
- Always create a new default environment:
 - conda create -n py37 python=3.7
 - conda activate py37
- Find packages:
 - conda search <package_name>
 - If list shows what you need:
 - conda install <package_name> (will also drag in dependencies)

Conda channels

- Channels are different locations/sources for packages.
- By default, an env is pointed to the default channel, you can confirm like so:
- The top-most channel has the highest priority for package searches.

```
$ conda config --show-sources
==> /Users/klay6683/.condarc <==
pinned_packages: []
report_errors: True
anaconda_upload: True
```

=> /Users/klay6683/miniconda3/envs/py37/.condarc <==
pinned_packages:</pre>

- conda-forge::bokeh
- conda-forge::opencv
- conda-forge::gdal
- conda-forge::numpy

channels:

- conda-forge
- defaults

Conda channels (2)

- What if you want to have one environment pointing to defaults and one to try out conda-forge?
 - -> ENV-dependent configuration!
- Activate the env you want to configure, then:
 - conda config --env --add channels conda-forge
- Good tip: Don't mix channels within one env. And pin packages to be sure.

Pinning packages

- Because conda sometimes finds "better" packages at default, conda did sometimes mix from different channels.
- To avoid this (catastrophic for gdal), pin packages per env to your desired channel:
 - conda config --env --add pinned_packages conda-forge::gdal

nb_conda_kernels

- If you are working mostly in Jupyter and (anticipate to) have more than one conda env, this is the most important conda package.
- It finds your existing conda envs at every launch of a Jupyter server
- It then offers kernel for each conda env in the list

- JNotebook: find menu "Kernel->change kernel"
- JLab: click on kernel name in the upper right



How to reinstall env in 5 min

- Even a "stable" env is rotting at some point
- The trick is to have:
 - File with a list of your conda packages
 - File with a list of your pip packages
 - If you develop new packages: file with a list of your own package folders and GH installs
 - a (couple of) bash script(s)

How to reinstall env in 5 min(2)

#!/bin/bash

. /Users/klay6683/miniconda3/etc/profile.d/conda.sh

```
if [ "$#" -ne 2 ]; then
    echo "Usage: $0 conda_env_name python_version_string (e.g. 3.7)" >&2
    exit 1
fi
if [ -n $CONDA_DEFAULT_ENV ]
then
    if [ "$CONDA_DEFAULT_ENV" == "$1" ]
    then
      echo "Deactive $1 environment first." >&2
    exit 1
    fi
fi
```

- conda deactivate
- ./reinstall_env.sh py37 3.7
- conda activate py37
- ./install_my_libs.sh

```
conda env remove -n "$1" -y
conda create -n "$1" -y -c conda-forge python="$2"
conda install -n "$1" -y -c conda-forge --file python_stuff/standard_py3_conda_packages.txt
```

1 ~	#!/bin/sh
2	# reinstall all my packages
3	cd ~/Dropbox/src
4 ~	<pre>for folder in 'pyciss' 'planet4' 'pyuvis' 'hirise_tools' 'nbtools' 'planetpy' 'pysis' 'p4terrains';</pre>
5	do cd \$folder;
6	<pre>echo "Installing \$folder";</pre>
7	echo;
8	pip install -e .;
9	cd ;
10	echo;
11	done
12	<pre># reinstall packages from pip that are needed</pre>
13	pip install -r pip_packages_to_install.txt
14	