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How to create and maintain a scientific Python environment using 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

Motivation

- Open Source science software is an extremely fast developing landscape

- The best new tools are often only a quick install away

- To "know Python" today also means to "know the available packages for your science domain and how to integrate them into your science environment"

- "Conda" has been extremely helpful with this task

- It allows you to quickly test out new packages without disturbing your "stable" environment.

Conda vs Anaconda vs Miniconda

- It's a bit of a word-jungle, so let's start with terminology to prevent confusion!

- Anaconda is first the name of the company that created the "conda" tool (more next slides)

- However, Anaconda is also the name of:

  - A Python science distribution targeted for beginners

  - The name of a meta-package (that lists other packages as requirement to be installed)

The conda executable

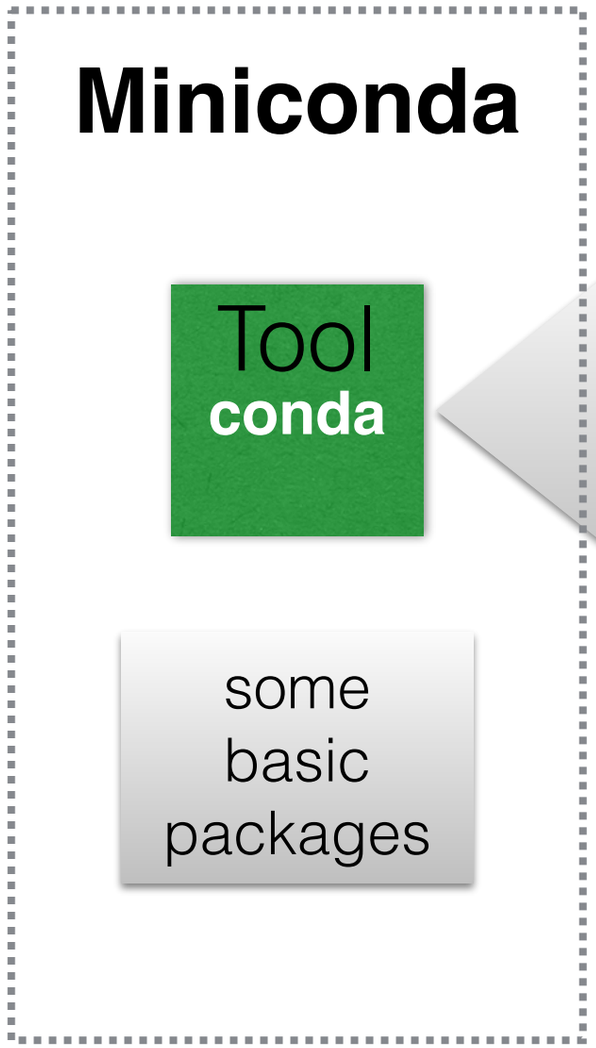
- Everything is centered around the *conda* executable.
- It's a command line tool
  - even when you manage your environments via the Anaconda Navigator GUI, this tool is running in the back
- Mostly used for managing Python things, but can do more:
  - conda also can install C/++/FORTRAN library dependencies for a given Python package (e.g. for SciPy, GDAL, OpenCV)
  - There are also a lot of R conda packages now

Conda tool (2)

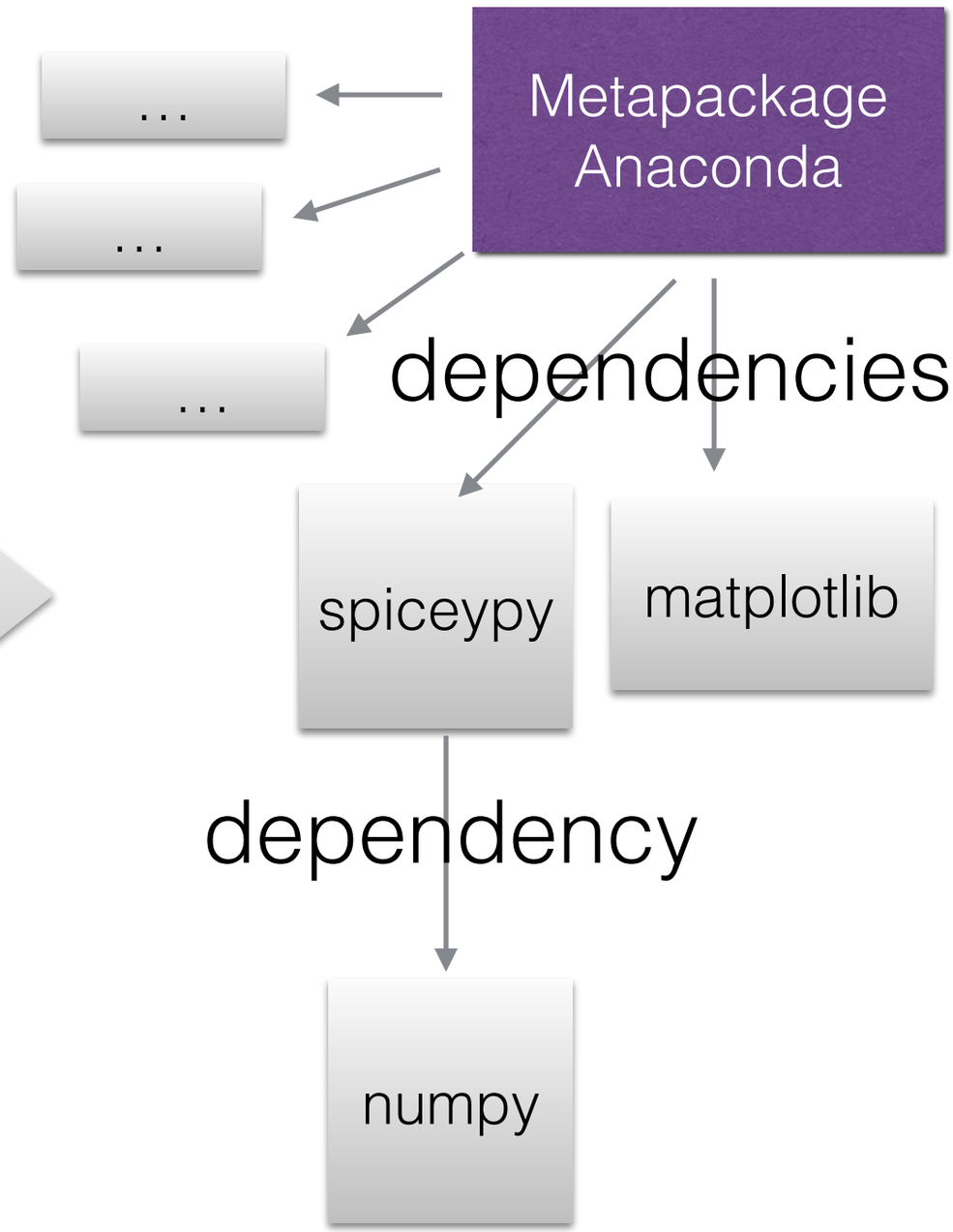
- With *conda* you should never need admin/root access for installing Python
  - Why? Because all the libraries can be installed into a folder of your home space
  - Additional pip-installs will also only install in there as well (If used correctly! More on that later!)

Conda vs Anaconda vs Miniconda (2)

Miniconda is a minimal set of pckgs, to be expanded by users that know what pckgs they need



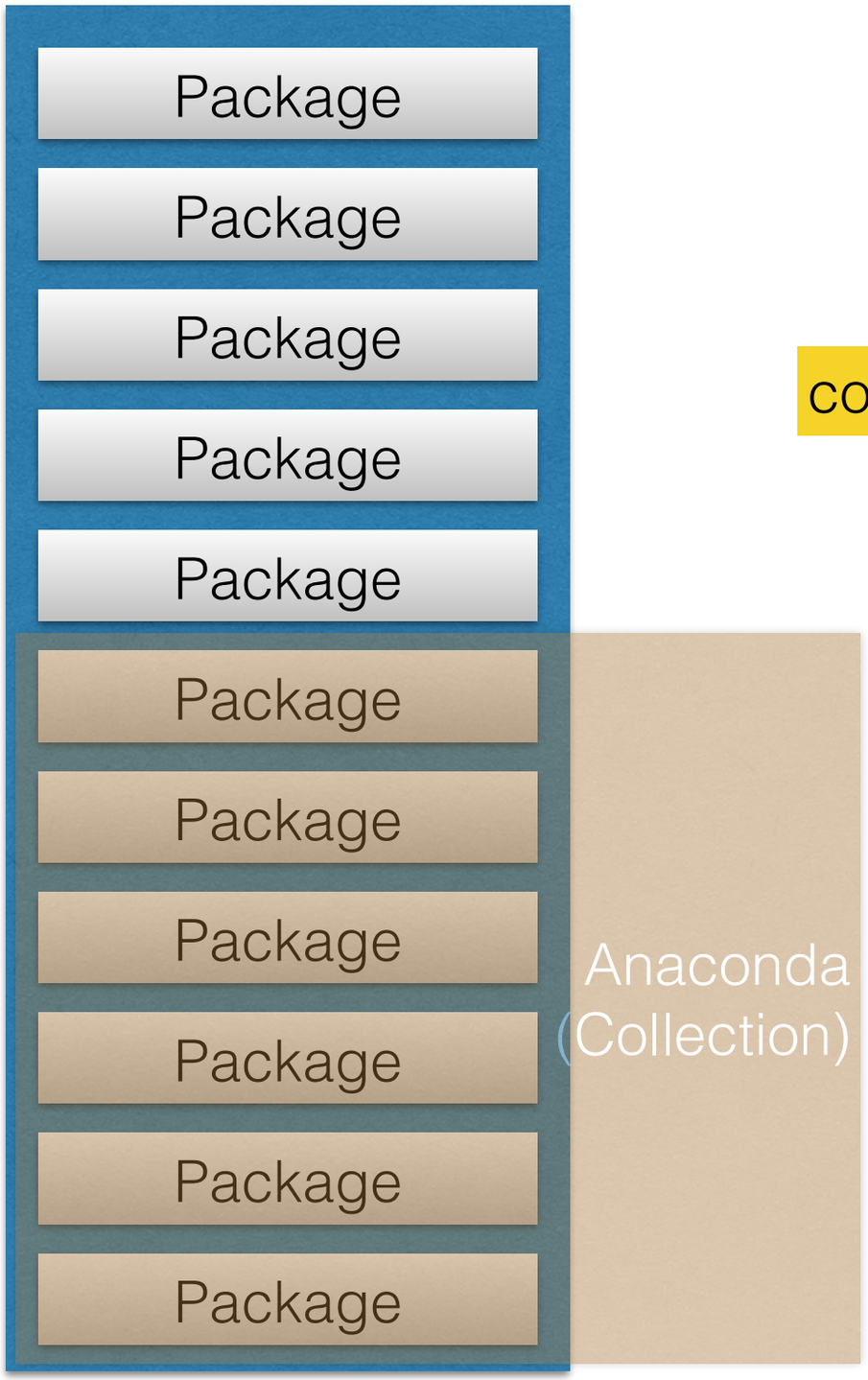
Anaconda: best for beginners



Standard conda package (grey)

conda create -n env_name python=3.8 pckg1 pckg2 ....

A conda environment



conda create -n env_name python=3.8 anaconda

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 know which packages you need for your use case.**
  - “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.**

Mamba!

- New faster drop-in replacement for conda
- In all conda commands you can replace "conda" by "mamba" if you have it installed.
- You can install already a mamba-installed version of conda envs using prepared installers from here:
- https://github.com/conda-forge/miniforge#mambaforge

conda environments

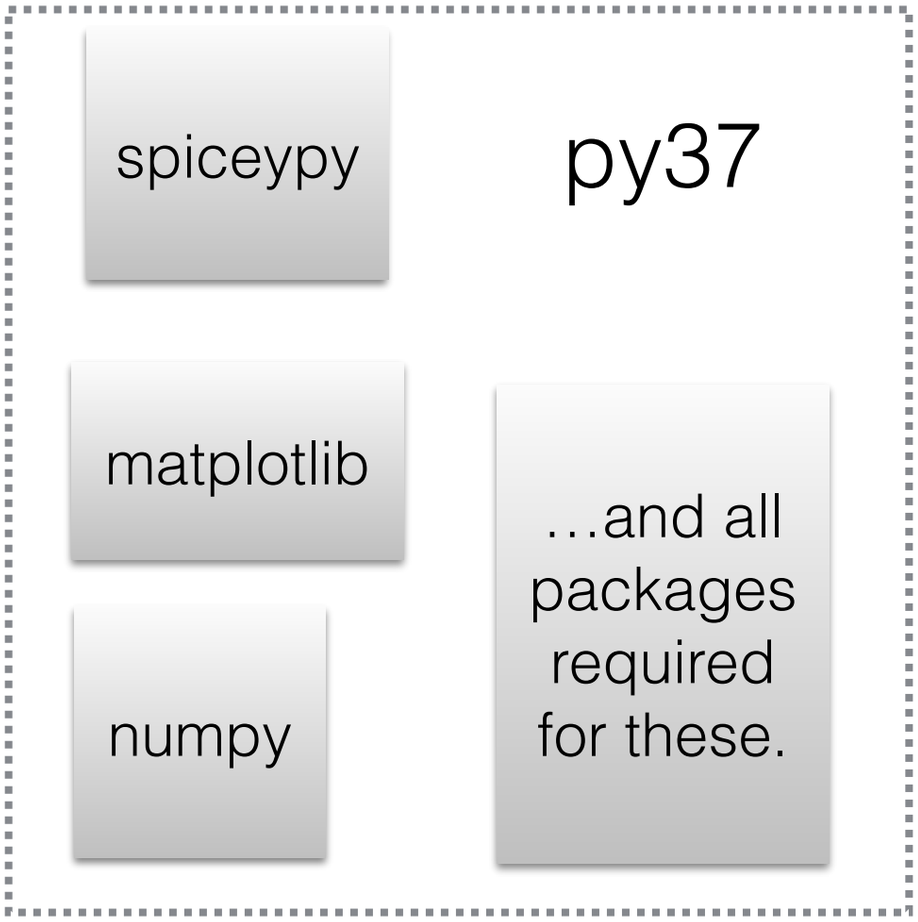
- conda's MO is based on (virtual) environments
- after installation, you have a "base" env.
    - if you still have an env named "root", I highly encourage you to wipe it all and reinstall
        - conda "suffered" from its own success:
            - rapid development led to breaking changes
            - these changes sometimes left incompatible remnants on your system
- same versions of pckgs are hardlinked between different envs, if possible
    - saves 50-70 % space, in my tests

Do you need envs?

- tl;dr : Yes
- Advanced (Python) hacking is NOT the criterium for using more than one env
- Not even "advanced Python usage" is.
- Piece of mind is the best criterium
    - ease of use is a supporting argument
- Why? Because the base environment is also the base for conda's functionality
    - That means, messing it up can render conda dysfunctional
        - -> reinstall of the whole ana/mini conda system might be required
    - While messing up one env (that isn't "base") only requires recreating the env

Creating envs

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.
    - Always watch what pip is doing! It has a summary of changes at the end.
- 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.... however ===>

The conda-pip frenemies

- pip is good; it checks dependencies as well, and makes sure that you get the dependencies AS DEFINED BY THE PACKAGE AUTHOR

- **pip is even recommended over "python setup.py install" for local (GitHub) package folders, because it keeps good records for uninstallation**
    - "cd package_folder; pip install ." # note the dot!

- **However, pip does NOT tell conda what it did**.

- If a package author says it requires a lib version lower than you have, pip will replace it with the older version

    - While conda still thinks the newer one is installed!

- Lemma: NEVER run pip in the base env

    - Corollary: You need envs! (proven theorem, or something like that...)

What if?

- So what do you do if pip replaced one library/package with an older version?
    - 1. pip uninstall pck_name
    - 2. conda install pck_name --force-reinstall
- If pip replaced several packages, i'd rather vote for env replacement
    - the dependency tree might be compromised beyond repair by conda

Summary of everyday conda 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.
- Advice: 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)

Keep your shell config clean

Below should be all there is related to conda in your shell config file (like .bashrc or similar)

```
# >>> conda initialize >>>
# !! Contents within this block are managed by 'conda init' !!
__conda_setup="$('/home/maye/miniconda3/bin/conda' 'shell.bash' 'hook' 2> /dev/null)"
if [ $? -eq 0 ]; then
    eval "$__conda_setup"
else
    if [ -f "/home/maye/miniconda3/etc/profile.d/conda.sh" ]; then
        . "/home/maye/miniconda3/etc/profile.d/conda.sh"
    else
        export PATH="/home/maye/miniconda3/bin:$PATH"
    fi
fi
unset __conda_setup
# <<< conda initialize <<<
```

Use this if you don't like the auto-activated environment:

```
conda config --set auto_activate_base false
```

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:
  - 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

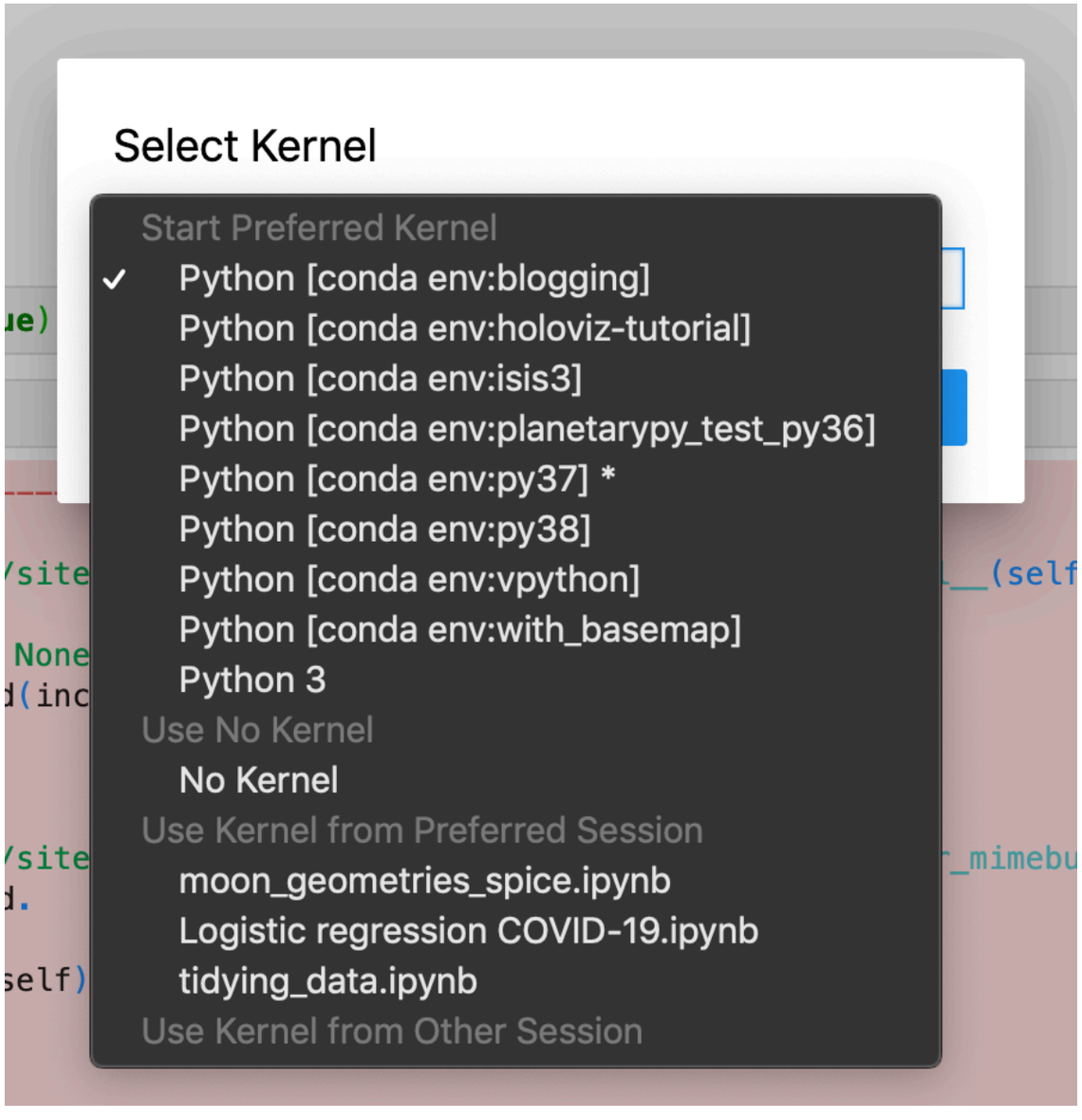
nb_conda_kernels

- 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 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
```

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

```
#!/bin/sh
# reinstall all my packages
cd ~/Dropbox/src
for folder in 'pyciss' 'planet4' 'pyuvis' 'hirise_tools' 'nbtools' 'planetpy' 'pysis' 'p4terrains';
    do cd $folder;
    echo "Installing $folder";
    echo;
    pip install -e .;
    cd .. ;
    echo;
done
# reinstall packages from pip that are needed
pip install -r pip_packages_to_install.txt

```

Today's recommendation

- Install a mamba-forge installer
  - It comes with mamba AND pre-configured conda-forge only channel

  - https://github.com/conda-forge/miniforge#mambaforge