Easy installations and virtual environments with conda

author: Maxime Borry date: 24/01/2020 width: 1440

Follow the presentation

maxibor.github.io/conda-presentation

What does it mean to install a program?

-> Copy/move the executable of the program in the PATH

What is the PATH?

```
borry@mpi-sdag1:~$ echo $PATH
/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/usr/
games:/usr/local/games:/opt/dell/srvadmin/bin
```

- /usr/local/sbin
- /usr/local/bin
- /usr/sbin
- /usr/bin
- . . .

When can't "install" programms on a computer, it's because you don't have write access to these directories

What's in my path?

For example, let's have a look at /usr/bin!

```
borry@mpi-sdag1:~$ ls -1 /usr/bin
...
head
headerdoc2html
heap
heap32
hexdump
hidutil
hiutil
host
...
```

Great, but what about Conda?

I have a confession: this is not my real path

```
borry@mpi-sdag1:~$ echo $PATH
/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/bin:/usr/
games:/usr/local/games:/opt/dell/srvadmin/bin
```

Here is my real path

```
borry@mpi-sdag1:~$ echo $PATH
/projects1/clusterhomes/borry/miniconda3/bin:/usr/local/
sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/usr/
games:/usr/local/games:/opt/dell/srvadmin/bin
```

The location where executables will be installed by Conda

/projects1/clusterhomes/borry/miniconda3/bin

Conda

"Conda is an open source, **cross-platform**, **language-agnostic package and environment management system** distributed by Continuum Analytics."

- Free
- No admin rights required
- Tons of bioinformatic packages available
- Easy to install

Install conda

Two distributions:

- Anaconda (fully featured, heavy)
- Miniconda (bare minimum)

Installation for Mac

```
borry@maxime:~$ wget https://repo.anaconda.com/miniconda/Miniconda3-latest-MacOSX-x86_64.sh -O ~/minicondaborry@maxime:~$ bash ~/miniconda.sh
```

Installation for Linux

```
borry@mpi-sdag1:~$ wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh -O ~/miniborry@maxime:~$ bash ~/miniconda.sh
```

Using conda

Install a package

When you install a package, conda automatically handles the installation of all its dependancies

Jupyter/IPython notebook

```
(base)borry@mpi-sdag1:~$ conda install jupyter
```

Install a package from a specific channel BWA

```
(base)borry@mpi-sdag1:~$ conda install -c bioconda bwa
```

Bioconda: Channel for bioinformatics packages

Bioconda: sustainable and comprehensive software distribution for the life sciences

conda-forge: community-led (huge) collection of recipes

Everything with conda is an environment

An environement is an isolated sandbox that allows a fine control on program's versions and dependancies

By default, you're in the base environment

```
(base)borry@mpi-sdag1:~$ conda env list
# conda environments:
#
base * /projects1/clusterhomes/borry/miniconda3
```

But can create new environments...

```
(base)borry@mpi-sdag1:~$ conda create -n myEnvName
```

Everything with conda is an environment(2)

Change your current environemnt (activate)

```
(base)borry@mpi-sdag1:~$ conda activate myEnvName
```

Note that your prompt now includes the name of the active environment

Install a package in this environment, for example, RStudio

```
(myEnvName) borry@mpi-sdag1:~$ conda install -c r rstudio
```

And go back to the base environment

```
(myEnvName) borry@mpi-sdag1:~$ conda deactivate
```

The packages installed in one environement are not accessible from outside!

Let's create an environment for MetaPhlan2 and Krona

Krona plots

```
(base)borry@mpi-sdag1:~$ conda create -n metaphlan
(base)borry@mpi-sdag1:~$ conda activate metaphlan
(metaphlan) borry@mpi-sdag1:~$ conda install -c bioconda metaphlan2

# Now you can use metaphlan !
(metaphlan) conda install -c bioconda krona
```

Now let's share our environement!

(metaphlan) borry@mpi-sdag1:~\$ conda env export > metaphlan_env.yml

And recreate it on another machine from the environment file

(base)borry@maxime:~\$ conda env create -f metaphlan_env.yml

Other useful conda commands

List installed packages and versions in an environment

(metaphlan) borry@mpi-sdag1:~\$ conda list

Uninstall a package (here Krona)

(metaphlan) borry@mpi-sdag1:~\$ conda remove krona

Delete an environment

(base)borry@mpi-sdag1:~\$ conda env remove -n metaphlan

Conda documentation: conda.io/docs