

### **Introduction to Conda**



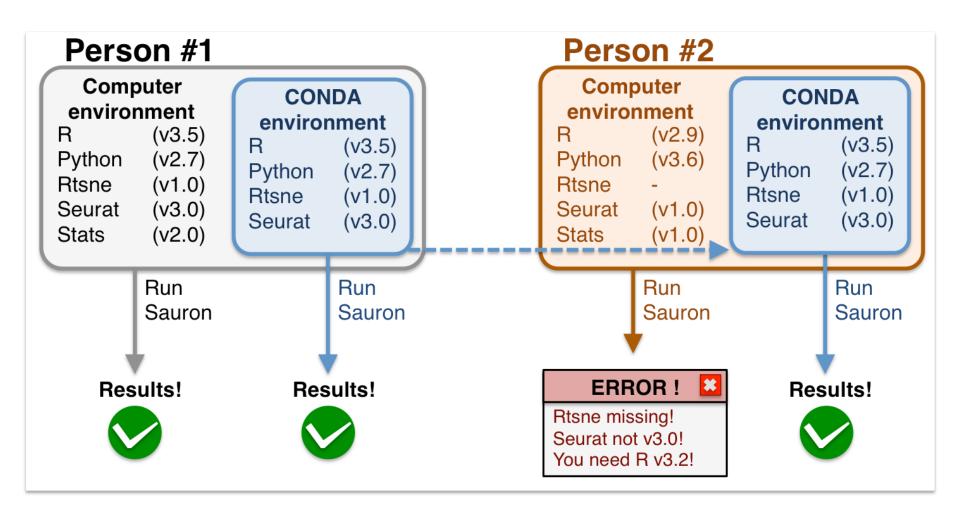
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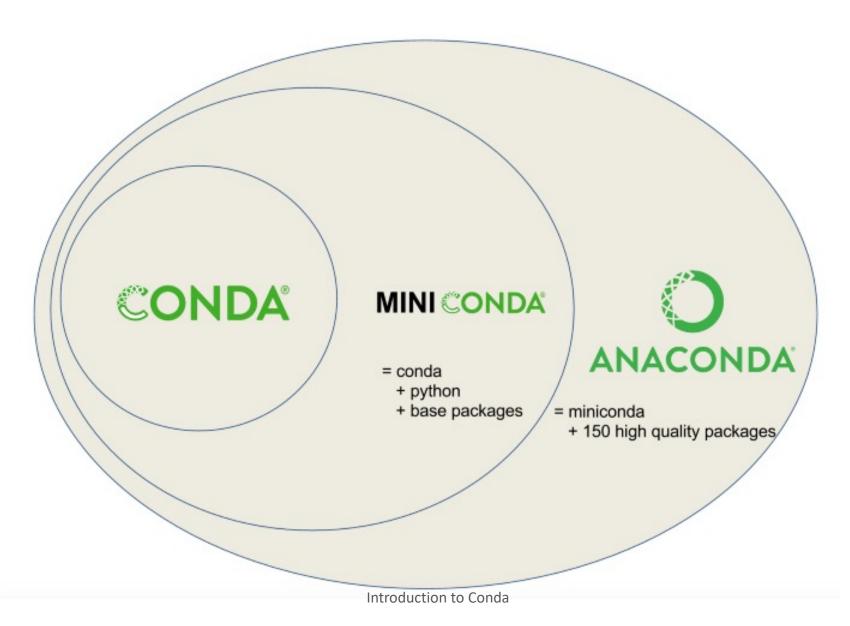
#### **Conda basics**



- Conda is an open source package and environment management system.
- It runs on Windows, Mac OS and Linux.
- Conda can quickly install, run, and update packages and dependencies.
- Conda can create, save, load, and switch between project specific software environments on your local computer.
- Conda was created for Python programs, but it can package and distribute software for any language.
- Do not require superuser privileges

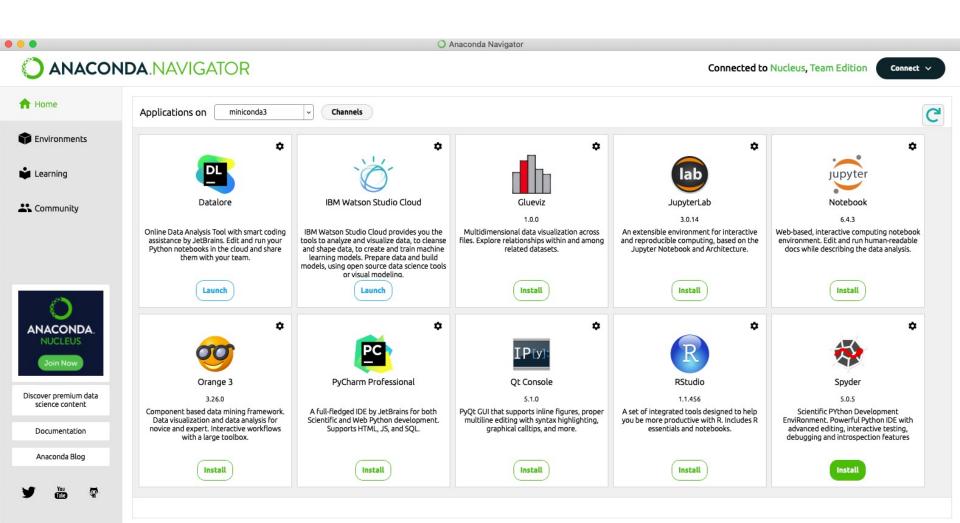






### **Anaconda navigator**

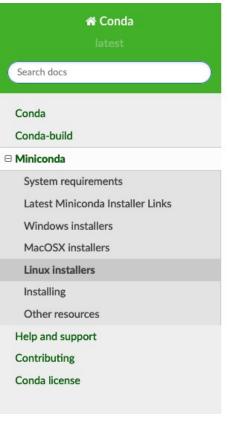




```
-bash-4.2$ conda create -y -n myenv python=3.8
 -bash-4.2$ conda activate myenv
 -bash-4.2$ conda install -y -n myenv -c bioconda bcftools
Collecting package metadata (current repodata.json): done
Solving environment: failed with initial frozen solve. Retrying with flexible solve.
Solving environment: failed with repodata from current repodata.json, will retry with next repodata source.
Collecting package metadata (repodata.json): done
Solving environment: failed with initial frozen solve. Retrying with flexible solve.
Solving environment: \
iled
 >>>>>>>>> PROR REPORT <
   Traceback (most recent call last):
     File "/root/anaconda3/lib/python3.7/site-packages/conda/cli/install.py", line 265, in install
       should_retry_solve=(_should_retry_unfrozen or repodata_fn != repodata_fns[-1]),
     File "/root/anaconda3/lib/python3.7/site-packages/conda/core/solve.py", line 117, in solve for transaction
       should retry solve)
     File "/root/anaconda3/lib/python3.7/site-packages/conda/core/solve.py", line 158, in solve for diff
       force remove, should retry solve)
     File "/root/anaconda3/lib/python3.7/site-packages/conda/core/solve.py", line 281, in solve final state
       ssc = self. run sat(ssc)
     File "/root/anaconda3/lib/python3.7/site-packages/conda/common/io.py", line 88, in decorated
       return f(*args, **kwds)
     File "/root/anaconda3/lib/python3.7/site-packages/conda/core/solve.py", line 808, in _run_sat
       should retry solve=ssc.should retry solve
     File "/root/anaconda3/lib/python3.7/site-packages/conda/common/io.py", line 88, in decorated
       return f(*args, **kwds)
     File "/root/anaconda3/lib/python3.7/site-packages/conda/resolve.py", line 1316, in solve
       raise UnsatisfiableError({})
   conda.exceptions.UnsatisfiableError:
   Did not find conflicting dependencies. If you would like to know which
```



### https://docs.conda.io/en/latest/miniconda.html#linux-installers



#### **Linux installers**

#### Linux

Python version	Name	Size	SHA256 hash	
Python 3.9	Miniconda3 Linux 64-bit	63.6 MiB	lea2f885b4dbc3098662845560bc64271eb17085387a70c2ba3f29fff6f8d52f	
	Miniconda3 Linux-aarch64 64-bit	62.6 MiB	4879820a10718743f945d88ef142c3a4b30dfc8e448d1ca08e019586374b773f	
	Miniconda3 Linux-ppc64le 64-bit	60.6 MiB	fa92ee4773611f58ed9333f977d32bbb64769292f605d518732183be1f3321fa	
	Miniconda3 Linux-s390x 64-bit	57.1 MiB	1faed9abecf4a4ddd4e0d8891fc2cdaa3394c51e877af14ad6b9d4aadb4e90d8	
Python 3.8	Miniconda3 Linux 64-bit	98.8 MiB	935d72deb16e42739d69644977290395561b7a6db059b316958d97939e9bdf3d	
	Miniconda3 Linux-aarch64 64-bit	94.8 MiB	19584b4fb5c0656e0cf9de72aaa0b0a7991fbd6f1254d12e2119048c9a47e5cc	
	Miniconda3 Linux-ppc64le 64-bit	93.3 MiB	c1ac79540cb77b2e0ca5b9f78b3bc367567d810118500a167dea4a0bcab5d063	
	Miniconda3 Linux-s390x 64-bit	89.0 MiB	55f514110a50e98549a68912cbb03e43a36193940a1889e1c8beb30009b4da19	
Python 3.7	Miniconda3 Linux 64-bit	84.9 MiB	a1a7285dea0edc430b2bc7951d89bb30a2a1b32026d2a7b02aacaaa95cf69c7c	
	Miniconda3 Linux-aarch64 64-bit	89.2 MiB	65f400a906e3132ddbba35a38d619478be77d32210a2acab05133d92ba08f111	
	Miniconda3 Linux-ppc64le 64-bit	88.1 MiB	e4f8b4a5eb8da1badf0b0c91fd7ee25e39120d4d77443e7a1ef3661fd439a997	
	Miniconda3 Linux-s390x 64-bit	84.1 MiB	7ab9f813dd84cb0951a2d755cd84708263ce4e03c656e65e2fa79ed0f024f0f7	



- -bash-4.2\$ mkdir -p ~/softwares/miniconda3
- -bash-4.2\$ cd ~/softwares/miniconda3
- -bash-4.2\$ wget https://repo.anaconda.com/miniconda/Miniconda3-py38\_4.10.3-Linux-x86\_64.sh
- -bash-4.2\$ chmod 775 Miniconda3-py38\_4.10.3-Linux-x86\_64.sh



# -bash-4.2\$ ./Miniconda3-latest-Linux-x86\_64.sh -b -p ~/softwares/miniconda3 –f

- -b run install in batch mode (without manual intervention), it is expected the license terms are agreed upon
- -f no error if install prefix already exists
- -h print this help message and exit
- **-p** PREFIX install prefix, defaults to /root/miniconda3, must not contain spaces.
- -s skip running pre/post-link/install scripts
- -u update an existing installation
- -t run package tests after installation (may install conda-build)



-bash-4.2\$ source ~/softwares/miniconda3/bin/activate

(base) -bash-4.2\$ conda init bash

(base) -bash-4.2\$ rm Miniconda3-latest-Linux-x86\_64.sh

### **Activating Conda Channels**



```
(base) -bash-4.2$ conda config --add channels defaults
(base) -bash-4.2$ conda config --add channels conda-forge
(base) -bash-4.2$ conda config --add channels anaconda
(base) -bash-4.2$ conda config --add channels bioconda
(base) -bash-4.2$ conda config --add channels biobuilds
(base) -bash-4.2$ conda config --add channels R
(base) -bash-4.2$ conda config --add channels intel
(base) -bash-4.2$ conda config --add channels trent
(base) -bash-4.2$ conda config --add channels plotly
```

#### List channels

(base) -bash-4.2\$ conda config --get channels

### Removing channels

(base) -bash-4.2\$ conda config --remove channels trent

### **Creating Conda Environments**



#### **Bioinformatics 1**

(base) -bash-4.2\$ conda create --yes --name bioinfo1 python=3.8 or

(base) -bash-4.2\$ conda create -y -n bioinfo1 python=3.8

#### **Bioinformatics 2**

(base) -bash-4.2\$ conda create -y -n bioinfo2 python=2.7

Deep learning

(base) -bash-4.2\$ conda create -y -n dl python=3.9

### **Creating Conda Environments**



#### R 3.6

(base) -bash-4.2\$ conda create -y -n r3.6 -c conda-forge r-base=3.6.3 r-essentials=3.6.0 python=3.8

#### R.4.1

(base) -bash-4.2\$ conda create -y -n r4.1 -c conda-forge r-base=4.1.0 r-essentials=4.1 python=3.8

### Switching Linear Algebra PACKage in Conda



#### R 4.1 (choose one library)

https://conda-forge.org/docs/maintainer/knowledge\_base.html?highlight

```
(base) -bash-4.2$ install -y -n r4.1 "libblas=*=*mkl"

(base) -bash-4.2$ install -y -n r4.1 "libblas=*=*openblas"

(base) -bash-4.2$ install -y -n r4.1 "libblas=*=*blis"

(base) -bash-4.2$ install -y -n r4.1 "libblas=*=*netlib"
```



# (base) -bash-4.2\$ conda env list

```
-bash-4.2$ conda env list
 conda environments:
base
                         /mnt/home/pelicion/softwares/miniconda3
Renv3.6
                         /mnt/home/pelicion/softwares/miniconda3/envs/Renv3.6
Renv4.0
                         /mnt/home/pelicion/softwares/miniconda3/envs/Renv4.0
aatk3
                         /mnt/home/pelicion/softwares/miniconda3/envs/gatk3
imputeme
                         /mnt/home/pelicion/softwares/miniconda3/envs/imputeme
ivdp
                         /mnt/home/pelicion/softwares/miniconda3/envs/ivdp
ivdp2
                         /mnt/home/pelicion/softwares/miniconda3/envs/ivdp2
r-env4.0
                         /mnt/home/pelicion/softwares/miniconda3/envs/r-env4.0
                         /mnt/home/pelicion/softwares/miniconda3/envs/sra
sra
```

### **Installing Conda Packages**



#### **Bioinformatics 1**

(base) -bash-4.2\$ conda install -y -n bioinfo1 —c bioconda gatk4 or

(base) -bash-4.2\$ conda install -y -n bioinfo1 —c bioconda gatk4=4.2.3.0

#### **Bioinformatics 2**

(base) -bash-4.2\$ conda install -y -n bioinfo2 -c bioconda platypus-variant

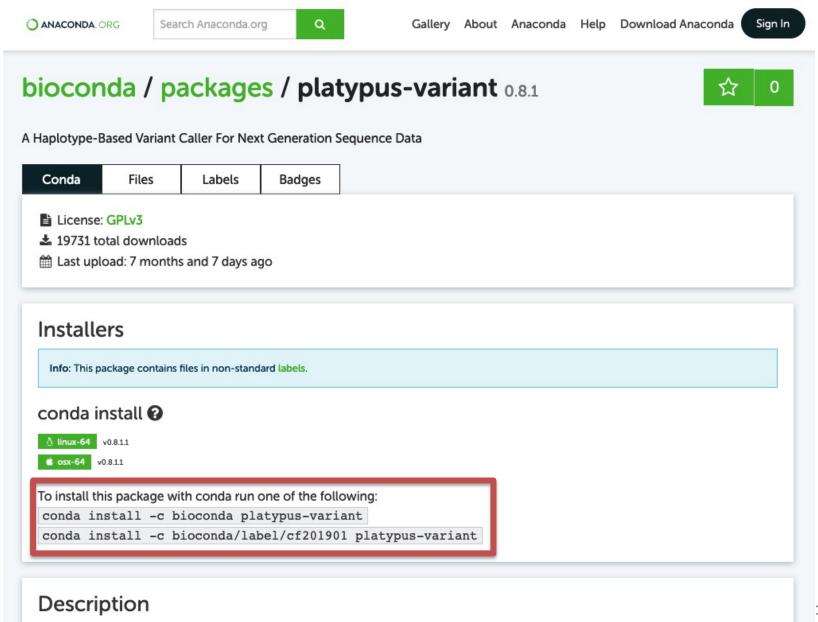


Q platypus variant caller + conda

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### Searching for packages







Q platypus variant caller + conda + recipe

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### **Searching for packages**



### BIOCONDA

#### Navigation

User Docs

Contributing to Bioconda

**Developer Docs** 

**Tutorials** 

Bioconda @ Github

Package Index



#### Quick search



# recipe platypus-variant

A Haplotype-Based Variant Caller For Next Generation Sequence Data

Homepage: http://www.well.ox.ac.uk/platypus

License: GPLv3

Recipe: /platypus-variant/meta.yaml

#### package platypus-variant

downloads 20k container none

Versions: 0.8.1.2-2, 0.8.1.2-1, 0.8.1.2-0, 0.8.1.1-3, 0.8.1.1-2,

0.8.1.1-1, 0.8.1.1-0, 0.8.1-1, 0.8.1-0

Depends: htslib<sup>O</sup> >=1.12,<1.13.0a0, libgcc-ng<sup>▼</sup> >=9.3.0,

python >=2.7,<2.8.0a0, python\_abi 2.7.\* \*\_cp27mu

Required By: • xyalign<sup>O</sup>

#### Installation

With an activated Bioconda channel (see 2. Set up channels), install with:

conda install platypus-variant

## **Searching for packages**



## (base) -bash-4.2\$ conda search r-base

r-base	4.0.3	ha43b4e8_3	conda-forge
r-base	4.0.3	hd23ff56_4	conda-forge
r-base	4.0.3	hd23ff56_5	conda-forge
r-base	4.0.3	hd23ff56_6	conda-forge
r-base	4.0.5	h8cab1ac_0	conda-forge
r-base	4.0.5	h9e01966_1	conda-forge
r-base	4.0.5	hb67fd72_2	conda-forge
r-base	4.0.5	hb93adac_3	conda-forge
r-base	4.1.0	h9e01966_0	conda-forge
r-base	4.1.0	h9e01966_1	conda-forge
r-base	4.1.0	hb67fd72_2	conda-forge
r-base	4.1.1	hb67fd72_0	conda-forge
r-base	4.1.1	hb93adac_1	conda-forge

### **Managing Conda Environments**



#### **Activate**

(base) -bash-4.2\$ conda activate bioinfo1 (bioinfo1) -bash-4.2\$

#### **Deactivate**

(bioinfo1) -bash-4.2\$ conda deactivate (base) -bash-4.2\$

#### **Activate and stack**

(base) -bash-4.2\$ conda activate bioinfo1 (bioinfo1) -bash-4.2\$ conda activate --stack r4.1 (r4.1) -bash-4.2\$

#### Removing an environment

(base) -bash-4.2\$ conda remove --n bioinfo2 --all

### **Managing Conda Environments**



### **Updating a package**

(base) -bash-4.2\$ conda update -n bioinfo1 gatk4

#### Removing a package

(base) -bash-4.2\$ conda remove -n bioinfo1 gatk4

or

(bioinfo1) -bash-4.2\$ conda remove gatk4

### **Sharing and Restoring Conda Environments**



### **Sharing an environment**

(base) -bash-4.2\$ conda env export -n bioinfo1 > bioinfo1.yml

### Sharing an environment across Mac OS, Windows, and Linux

(base) -bash-4.2\$ conda env export -n bioinfo1 --from-history > bioinfo1\_fh.yml

#### Creating an environment from an .yml file

(base) -bash-4.2\$ conda env create -f bioinfo1.yml



- https://github.com/rodrigopsav/conda
- pelicion@msu.edu
- rodrigopsa@yahoo.com