

# Introduction to Conda

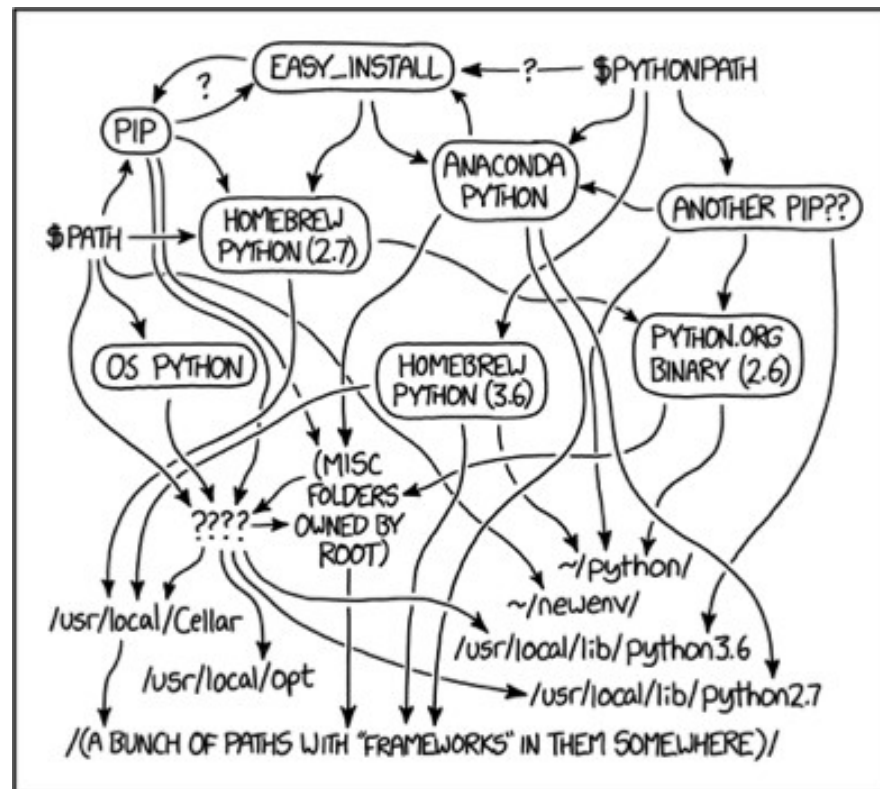
# Learning Outcomes

On successful completion of this module, students should be able to:

- **Use Docker, (bio)conda, and git to create reproducible analysis environments and generate reproducible results**
- Use the Linux command line environment including access/use of a High-Performance Compute (HPC) cluster
- Write Rmarkdown documents to generate reproducible research reports
- Analyse gene expression microarrays in order to identify differentially expressed genes, enriched GO terms, pathways, and gene sets
- Develop simple Shiny applications

# What is a Package Manager?

- Software to automate process of installing, upgrading, configuring, removing, applications/programs in a *consistent* manner



- Common Linux package managers include apt, snap, ppa dpkg, yum, rpm etc.

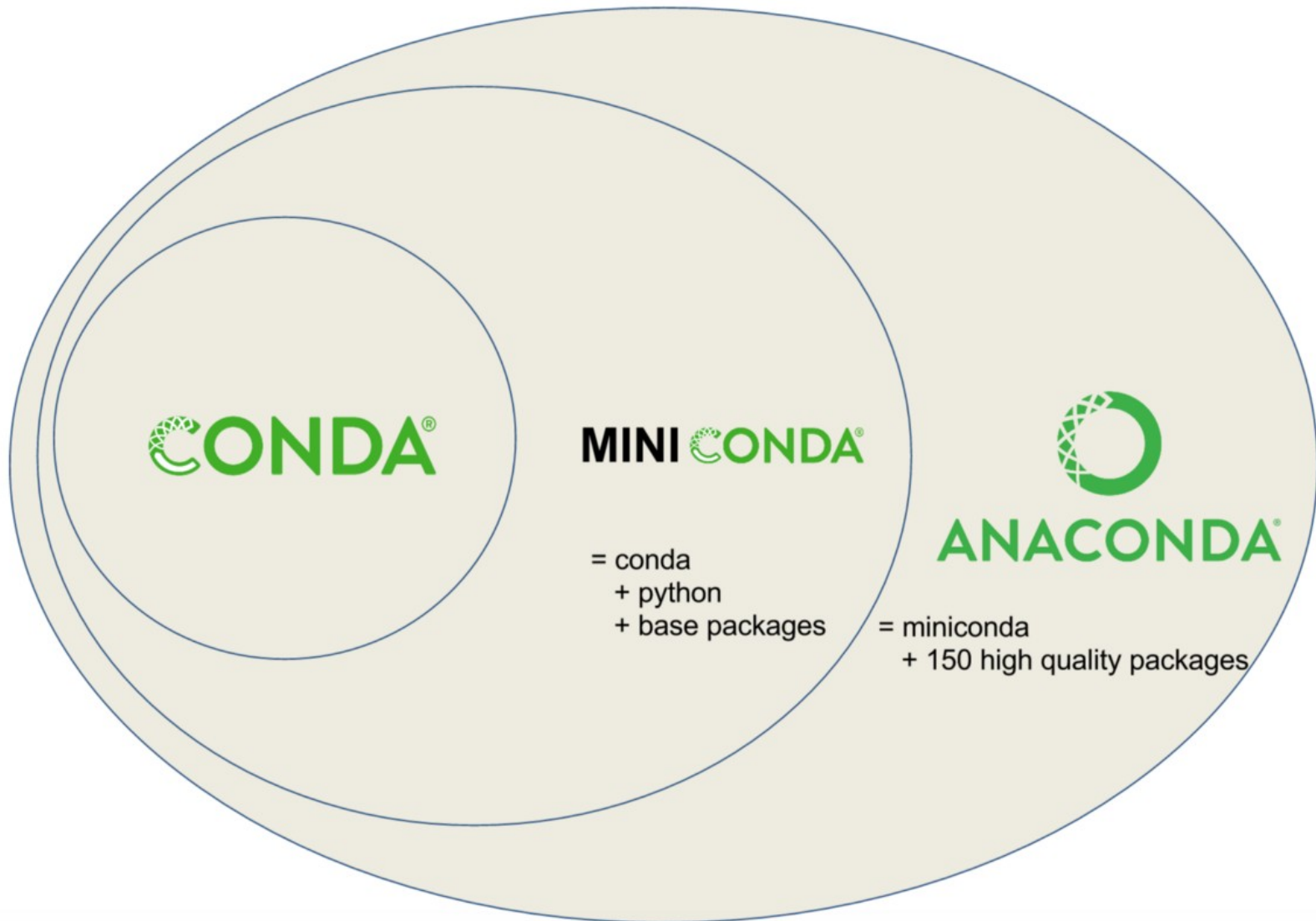
# What is Conda?

Package, dependency and environment management for any language

*“Conda is an open source package management system and environment management system that runs on Windows, macOS and Linux. Conda quickly installs, runs and updates packages and their dependencies. Conda easily creates, saves, loads and switches between environments on your local computer. It was created for Python programs, but it can package and distribute software for any language.”*

from: <https://conda.io/docs/>

# What is Miniconda / Anaconda?



# What is Miniconda / Anaconda?



Most Trusted Distribution for Data Science

## ANACONDA NAVIGATOR

Desktop Portal to Data Science

## ANACONDA PROJECT

Portable Data Science Encapsulation

## DATA SCIENCE LIBRARIES

### Data Science IDEs



### Analytics & Scientific Computing



### Visualization



### Machine Learning

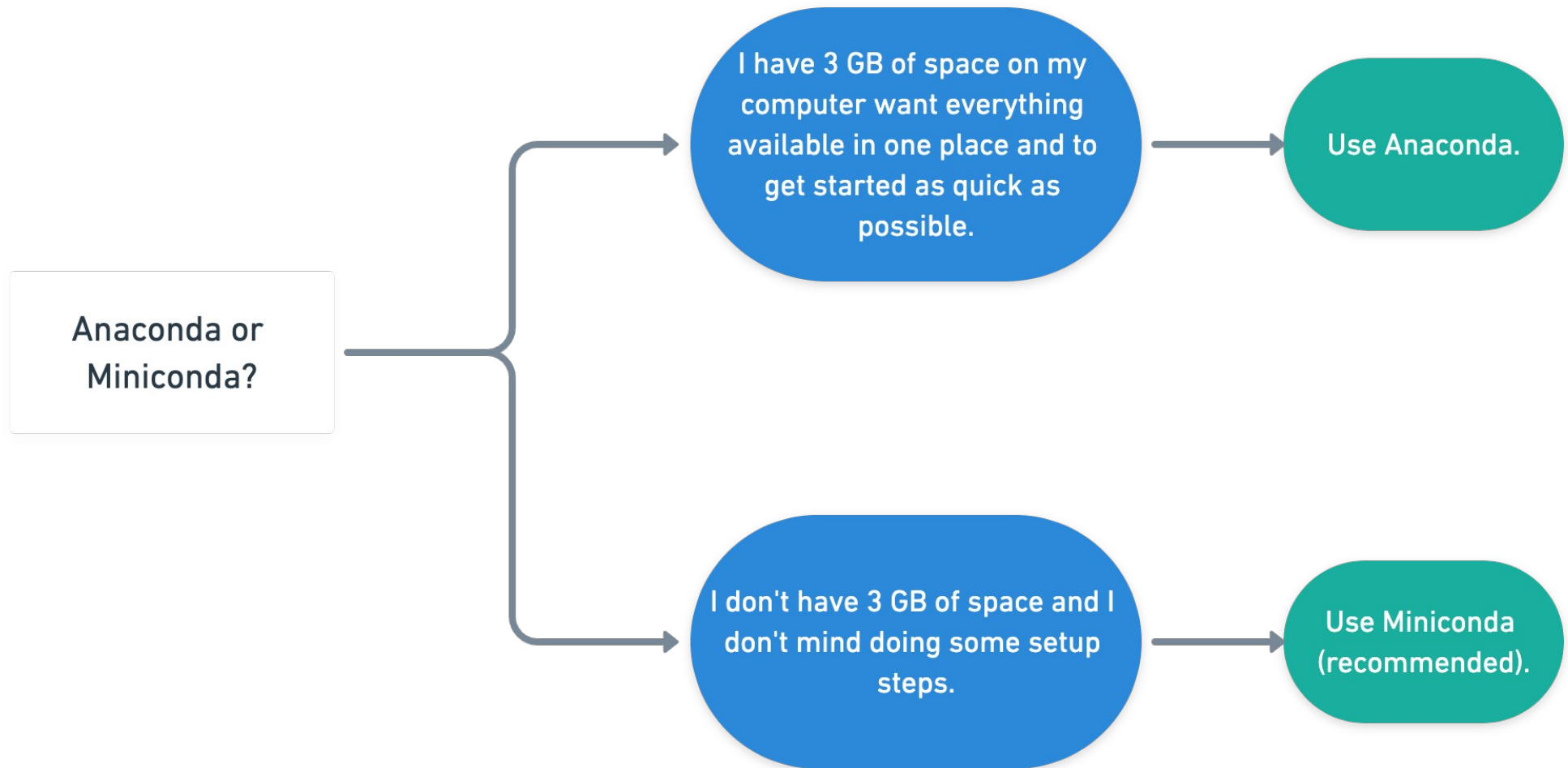


...and many more!

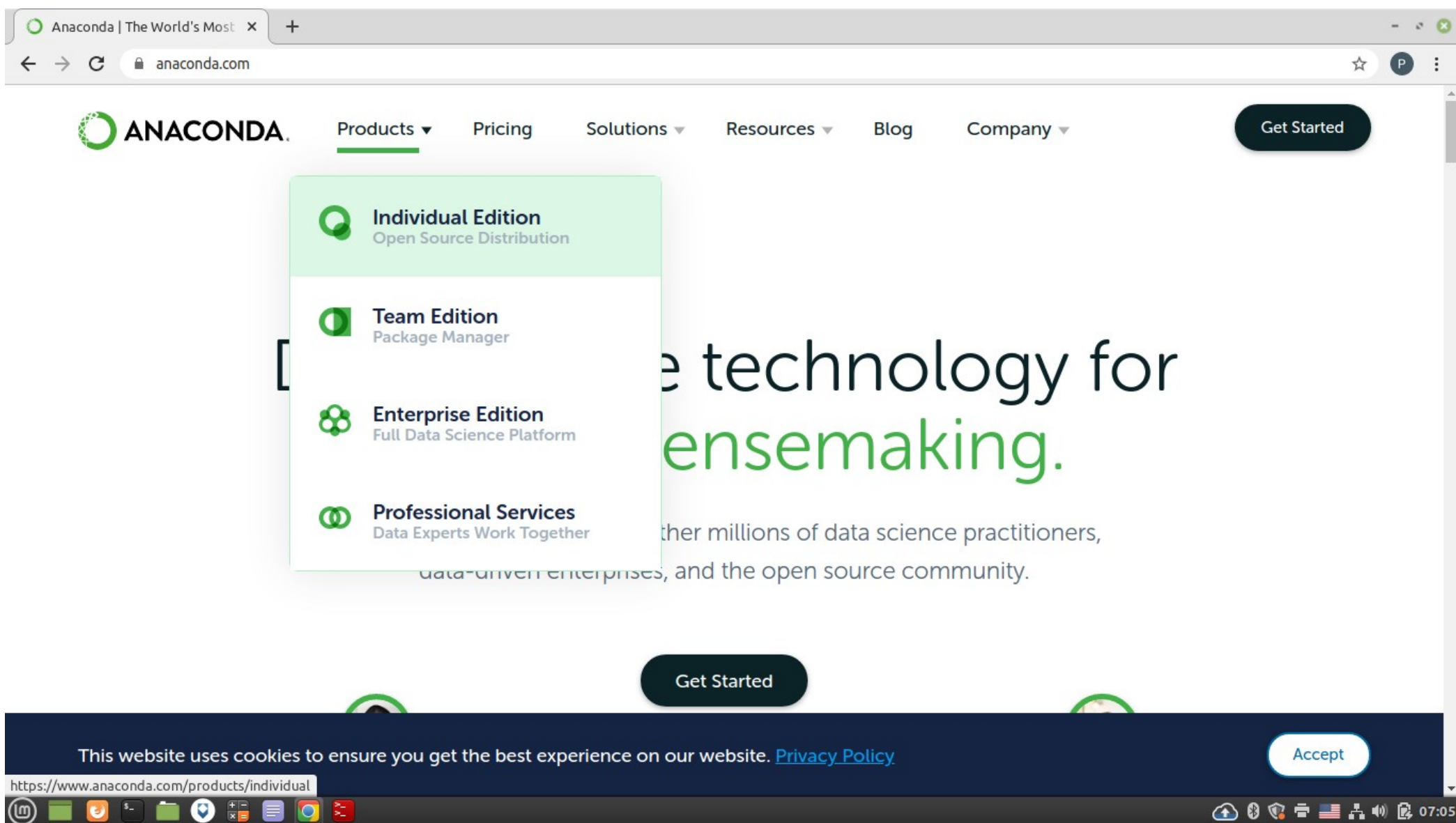


Data Science Package & Environment Manager

# What is Miniconda / Anaconda?



# Installing Anaconda



The screenshot shows the Anaconda website with the 'Products' dropdown menu open. The menu lists four options: Individual Edition (Open Source Distribution), Team Edition (Package Manager), Enterprise Edition (Full Data Science Platform), and Professional Services (Data Experts Work Together). The background features a large heading 'The technology for ensemaking.' and a 'Get Started' button. A cookie consent banner is visible at the bottom.

Anaconda | The World's Most x +

anaconda.com

ANACONDA. Products Pricing Solutions Resources Blog Company Get Started

- Individual Edition  
Open Source Distribution
- Team Edition  
Package Manager
- Enterprise Edition  
Full Data Science Platform
- Professional Services  
Data Experts Work Together

The technology for ensemaking.

ther millions of data science practitioners,  
data-driven enterprises, and the open source community.

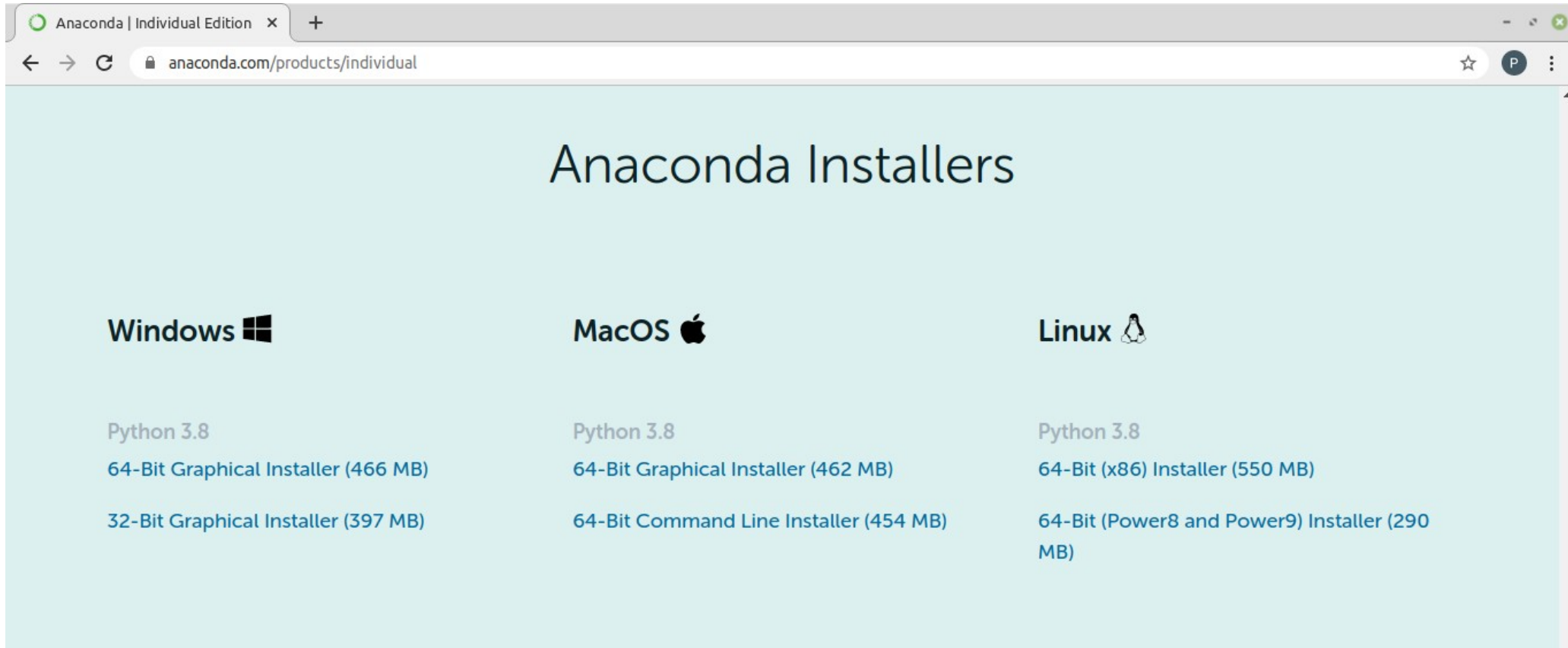
Get Started

This website uses cookies to ensure you get the best experience on our website. [Privacy Policy](#) Accept

https://www.anaconda.com/products/individual



# Installing Anaconda



The screenshot shows a web browser window with the address bar displaying 'anaconda.com/products/individual'. The page title is 'Anaconda | Individual Edition'. The main heading is 'Anaconda Installers'. Below this, there are three columns for different operating systems: Windows, MacOS, and Linux. Each column lists the Python version (3.8) and the available installers with their sizes.

Operating System	Python Version	Installer Type	Size
Windows	Python 3.8	64-Bit Graphical Installer	466 MB
		32-Bit Graphical Installer	397 MB
MacOS	Python 3.8	64-Bit Graphical Installer	462 MB
		64-Bit Command Line Installer	454 MB
Linux	Python 3.8	64-Bit (x86) Installer	550 MB
		64-Bit (Power8 and Power9) Installer	290 MB

# Installing Anaconda

```
pilib@kari: ~/Desktop
File Edit View Search Terminal Help
pilib@kari:~/Desktop$ chmod a+x Anaconda3-2020.07-Linux-x86_64.sh
pilib@kari:~/Desktop$ ./Anaconda3-2020.07-Linux-x86_64.sh

Welcome to Anaconda3 2020.07

In order to continue the installation process, please review the license
agreement.
Please, press ENTER to continue
>>> 
```

```
Do you accept the license terms? [yes|no]
[no] >>> yes
```

```
Anaconda3 will now be installed into this location:
/home/pilib/anaconda3
```

- Press ENTER to confirm the location
- Press CTRL-C to abort the installation
- Or specify a different location below

```
[/home/pilib/anaconda3] >>> 
```



# Installing Anaconda

```
watchdog          pkgs/main/linux-64::watchdog-0.10.3-py38_0
wcwidth           pkgs/main/noarch::wcwidth-0.2.5-py_0
webencodings      pkgs/main/linux-64::webencodings-0.5.1-py38_1
werkzeug          pkgs/main/noarch::werkzeug-1.0.1-py_0
wheel             pkgs/main/linux-64::wheel-0.34.2-py38_0
widgetsnbextension pkgs/main/linux-64::widgetsnbextension-3.5.1-py38_0
wrapit            pkgs/main/linux-64::wrapit-1.11.2-py38h7b6447c_0
wurlitzer         pkgs/main/linux-64::wurlitzer-2.0.1-py38_0
xlrd              pkgs/main/noarch::xlrd-1.2.0-py_0
xlsxwriter        pkgs/main/noarch::xlsxwriter-1.2.9-py_0
xlwt              pkgs/main/linux-64::xlwt-1.3.0-py38_0
xmldict           pkgs/main/noarch::xmldict-0.12.0-py_0
xz                pkgs/main/linux-64::xz-5.2.5-h7b6447c_0
yaml              pkgs/main/linux-64::yaml-0.2.5-h7b6447c_0
yapf              pkgs/main/noarch::yapf-0.30.0-py_0
zeromq            pkgs/main/linux-64::zeromq-4.3.2-he6710b0_2
zict              pkgs/main/noarch::zict-2.0.0-py_0
zipp              pkgs/main/noarch::zipp-3.1.0-py_0
zlib              pkgs/main/linux-64::zlib-1.2.11-h7b6447c_3
zope              pkgs/main/linux-64::zope-1.0-py38_1
zope.event        pkgs/main/linux-64::zope.event-4.4-py38_0
zope.interface    pkgs/main/linux-64::zope.interface-4.7.1-py38h7b6447c_0
zstd              pkgs/main/linux-64::zstd-1.4.5-h0b5b093_0
```

Preparing transaction: done

Executing transaction: done

installation finished.

Do you wish the installer to initialize Anaconda3  
by running conda init? [yes|no]

# Installing Anaconda

```
pilib@kari:~$ conda info
```

```
active environment : None
  shell level      : 0
  user config file  : /home/pilib/.condarc
populated config files : /home/pilib/.condarc
  conda version     : 4.8.3
  conda-build version : 3.18.11
  python version     : 3.8.3.final.0
  virtual packages   : __glibc=2.31
  base environment   : /home/pilib/anaconda3 (writable)
    channel URLs     : 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/pilib/anaconda3/pkgs
                      /home/pilib/.conda/pkgs
  envs directories   : /home/pilib/anaconda3/envs
                      /home/pilib/.conda/envs
    platform         : linux-64
    user-agent        : conda/4.8.3 requests/2.24.0 CPython/3.8.3
31
    UID:GID          : 1000:1000
    netrc file        : None
    offline mode      : False
```

```
pilib@kari:~$ conda -V
conda 4.8.3
```

# Updating Anaconda

**conda update --prefix /path/to/anaconda3 anaconda**

```
pilib@kari:~$ conda update --prefix /home/pilib/anaconda3 anaconda
Collecting package metadata (current_repodata.json): done
Solving environment: done
```

```
## Package Plan ##
```

```
environment location: /home/pilib/anaconda3
```

```
added / updated specs:
- anaconda
```

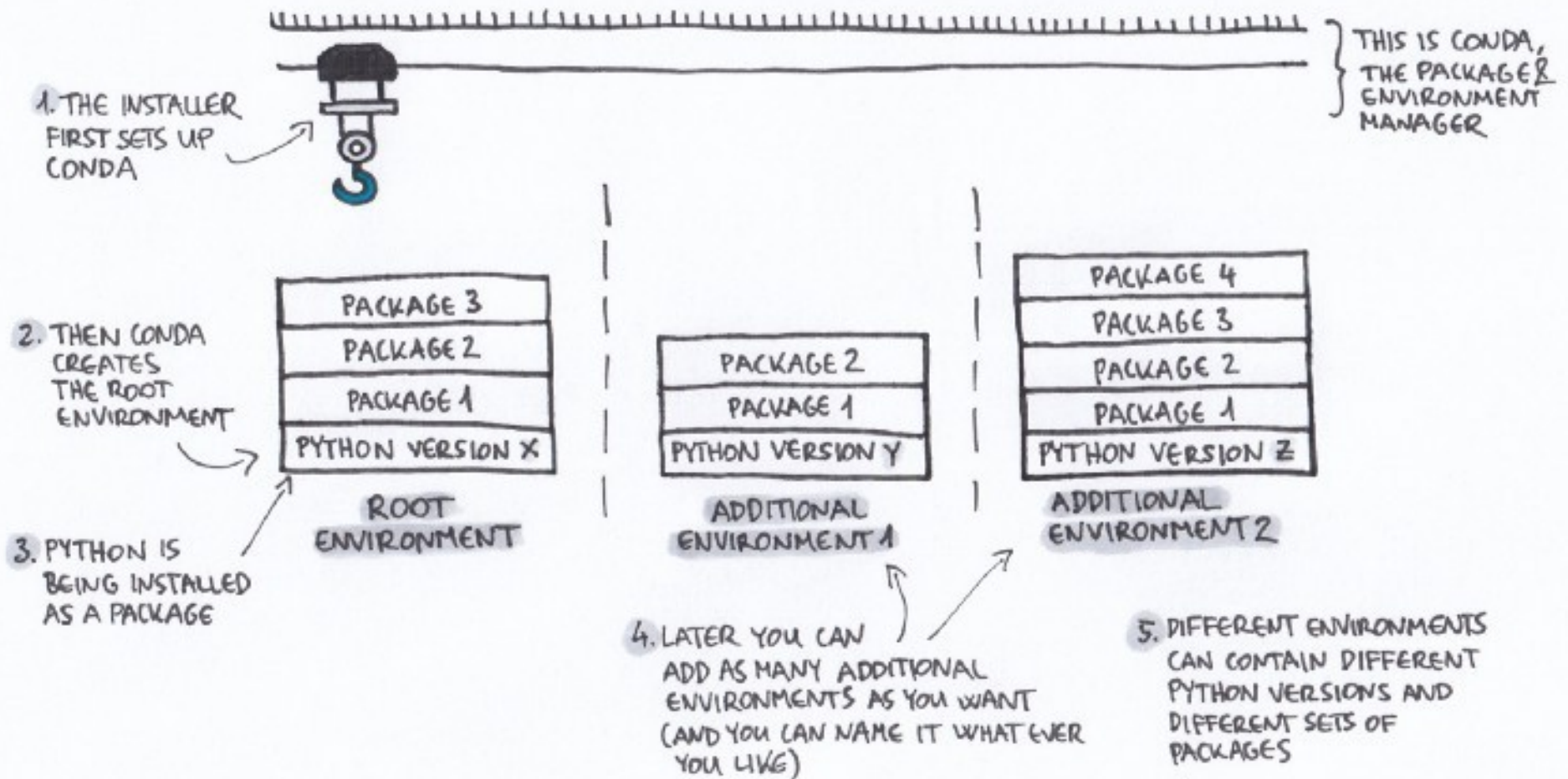
The following packages will be downloaded:

package	build	
-----	-----	
_anaconda_depends-2020.07	py38_0	6 KB
anaconda-custom	py38_1	35 KB
argon2-cffi-20.1.0	py38h7b6447c_1	46 KB
asn1crypto-1.4.0	py_0	80 KB
async_generator-1.10	py_0	24 KB
attrs-20.2.0	py_0	42 KB
autopep8-1.5.4	py_0	42 KB
bitarray-1.5.3	py38h7b6447c_0	93 KB
bleach-3.2.1	py_0	112 KB
blosc-1.20.0	hd408876_0	71 KB
bokeh-2.2.1	py38_0	5.4 MB
ca-certificates-2020.7.22	_0	125 KB
cffi-1.14.3	py38he30daa8_0	225 KB



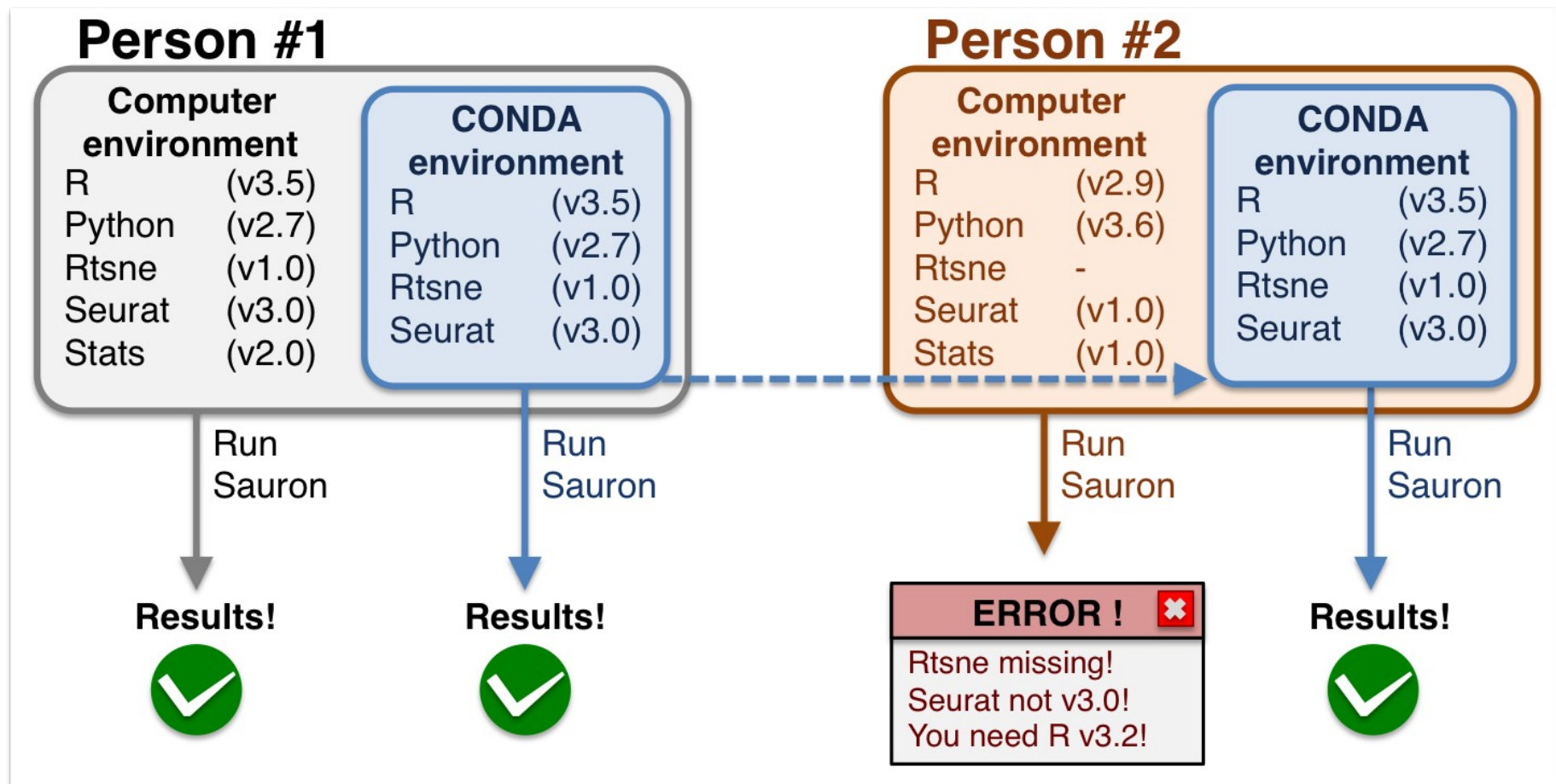
# Conda Environments

- Environment = a specific collection of conda packages you have installed.  
Can **create**, **list**, **config**, **update**, **remove**, and **export** environments



# Conda Environments

- Environment = a specific collection of conda packages you have installed.  
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# Managing Environments

<b>conda env list</b>	# list all environments (* = current)
<b>conda create -- name test</b>	# create new env called test
<b>conda activate test</b>	# switch to this new environment

```
pilib@kari:~$ conda create --name test
Collecting package metadata (current_repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /home/pilib/anaconda3/envs/test

Proceed ([y]/n)? y

Preparing transaction: done
Verifying transaction: done
Executing transaction: done
#
# To activate this environment, use
#
#     $ conda activate test
#
# To deactivate an active environment, use
#
#     $ conda deactivate
```



# Managing Packages

**conda list**

# List packages in active env

**conda search pkgname**

# Search for package

**conda install pkgname=ver**

# Install specific package version

**conda update pkgname**

# Update package

```
pilib@kari:~$ conda activate test
(test) pilib@kari:~$ conda list
# packages in environment at /home/pilib/anaconda3/envs/test:
#
# Name                                Version                                Build    Channel
(test) pilib@kari:~$ conda search python
Loading channels: done
# Name                                Version                                Build    Channel
python                                2.7.13                                hac47a24_15 pkgs/main
python                                2.7.13                                heccc3f1_16 pkgs/main
python                                2.7.13                                hfff3488_13 pkgs/main
python                                2.7.14                                h1571d57_29 pkgs/main
python                                2.7.14                                h1571d57_30 pkgs/main
python                                2.7.14                                h1571d57_31 pkgs/main
python                                2.7.14                                h1aa7481_19 pkgs/main
python                                2.7.14                                h435b27a_18 pkgs/main
```

# Managing Packages

```
python 3.8.3 hcff3b4d_0 pkgs/main
python 3.8.3 hcff3b4d_2 pkgs/main
python 3.8.5 h7579374_1 pkgs/main
python 3.8.5 hcff3b4d_0 pkgs/main
(test) pilib@kari:~$ conda install python=2.7.14
Collecting package metadata (current_repodata.json): done
Solving environment: failed with initial frozen solve. Retrying with flexible solve.
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /home/pilib/anaconda3/envs/test

  added / updated specs:
    - python=2.7.14
```

```
(test) pilib@kari:~$ python
Python 2.7.14 |Anaconda, Inc.| (default, Mar 27 2018, 17:29:31)
[GCC 7.2.0] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> █
```

# Managing Channels

- Conda channels are repositories – collections of software

**conda config --add channels CHANNELNAME**

**conda install CHANNELNAME::PKGNAME**

bioconda.github.io

**BIOCONDA**<sup>®</sup>

Navigation

- User Docs
- Contributing to Bioconda
- Developer Docs
- Tutorials
- Bioconda @ Github
- Package Index
- chat on gitter

Quick search

**BIOCONDA**<sup>®</sup>

Bioconda is a channel for the [conda](#) package manager specializing in bioinformatics software. Bioconda consists of:


- a [repository of recipes](#) hosted on GitHub
- a [build system](#) turning these recipes into conda packages
- a [repository of packages](#) containing over 7000 bioinformatics packages ready to use with `conda install`
- over 850 contributors and 570 members who add, modify, update and maintain the recipes

The conda package manager makes installing software a vastly more streamlined process. Conda is a combination of other package managers you may have

**conda search --channel bioconda**

**conda search --channel bioconda | wc -l**

# Anaconda Navigator



Sign in to Anaconda Cloud

Home

Environments

Projects (beta)

Learning


Community

Documentation

Developer Blog

Feedback


Applications on root Channels Refresh



jupyter  
notebook  
5.0.0

Web-based, interactive computing notebook environment. Edit and run human-readable docs while describing the data analysis.


Launch



IP[y]  
qtconsole  
4.3.0

PyQt GUI that supports inline figures, proper multiline editing with syntax highlighting, graphical calltips, and more.

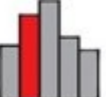
Launch



spyder  
3.1.4

Scientific PYTHON Development Environment. Powerful Python IDE with advanced editing, interactive testing, debugging and introspection features


Launch



glueviz  
0.10.4

Multidimensional data visualization across files. Explore relationships within and among related datasets.


Install



orange3  
3.4.1

Component based data mining framework. Data visualization and data analysis for novice and expert. Interactive workflows with a large toolbox.

Install



R  
rstudio  
1.0.136

A set of integrated tools designed to help you be more productive with R. Includes R essentials and notebooks.

Install