Introduction to Conda

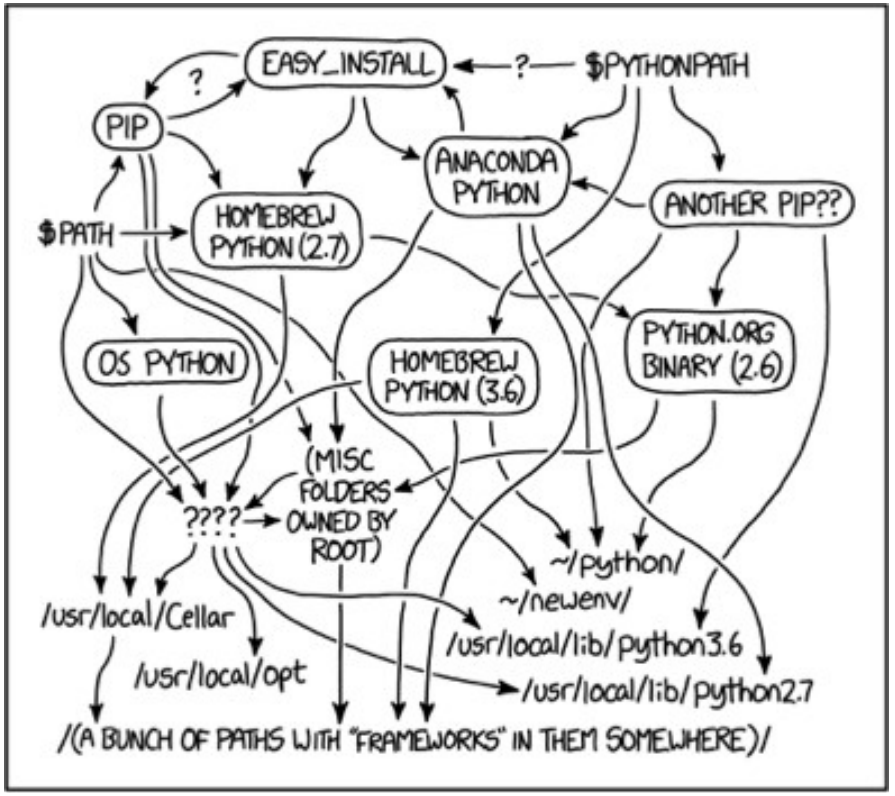
Learning Outcomes

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 mangers include apt, snap, ppa dpkg, yum, rpm etc.

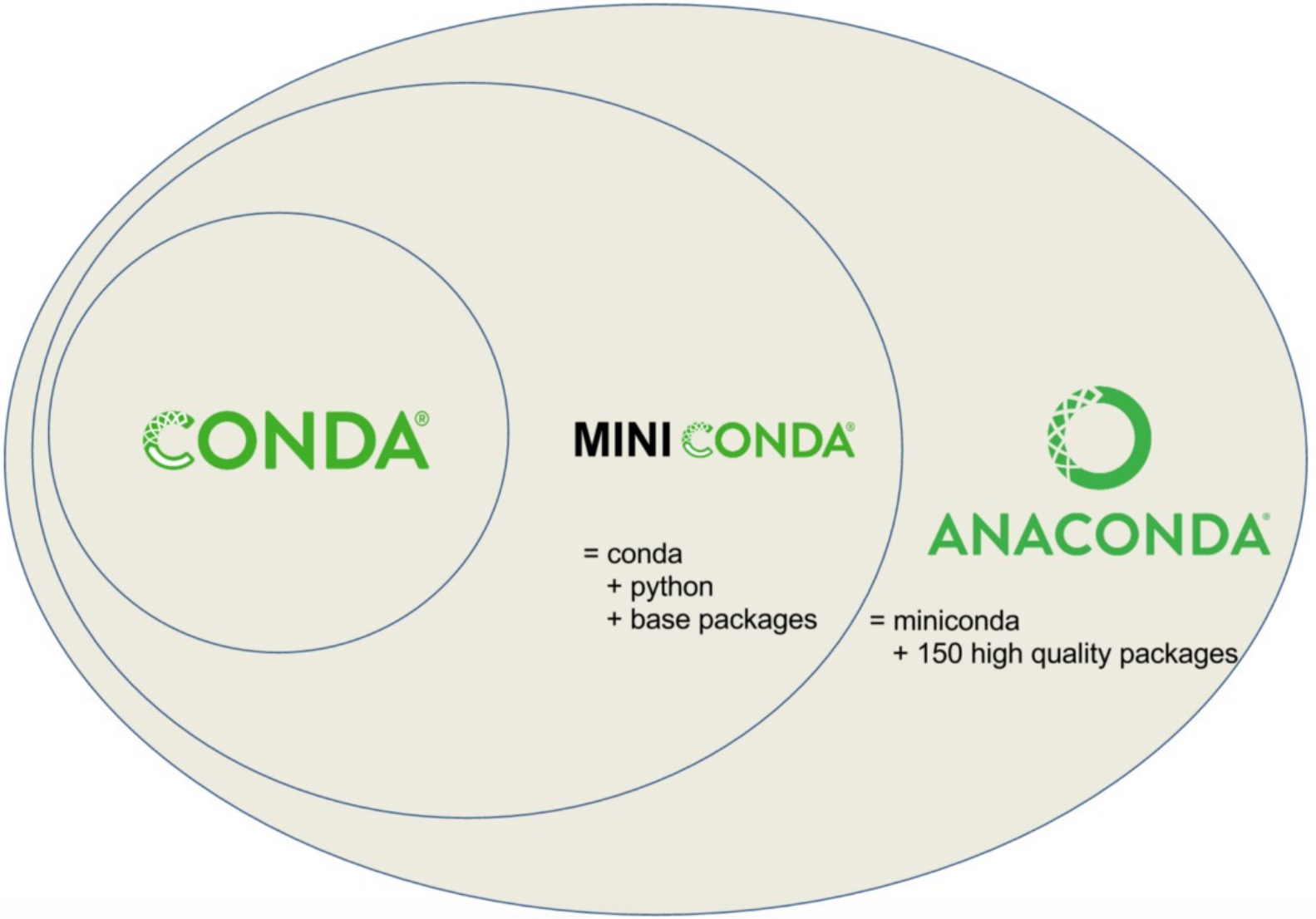
What is Conda?

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?



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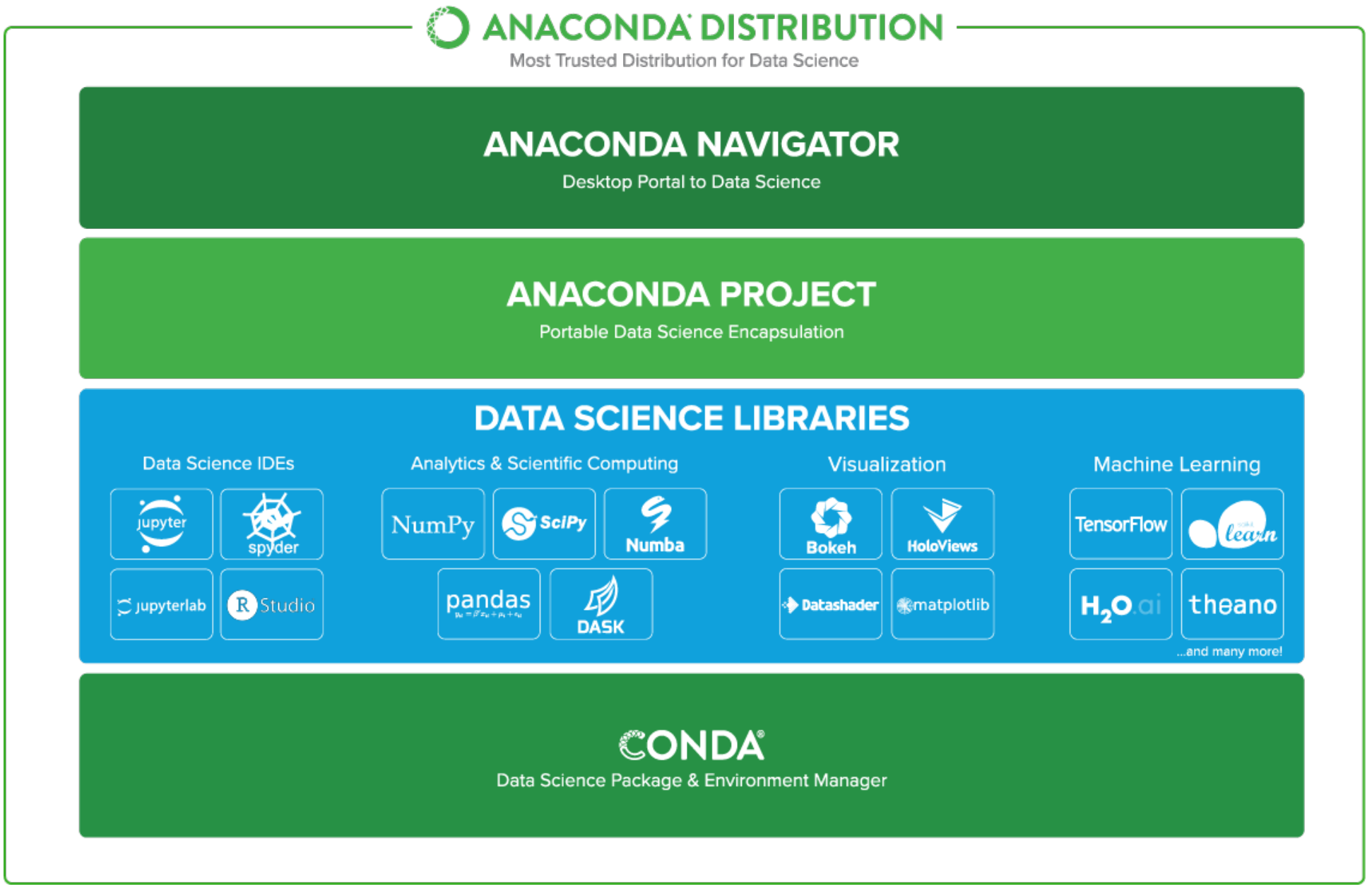

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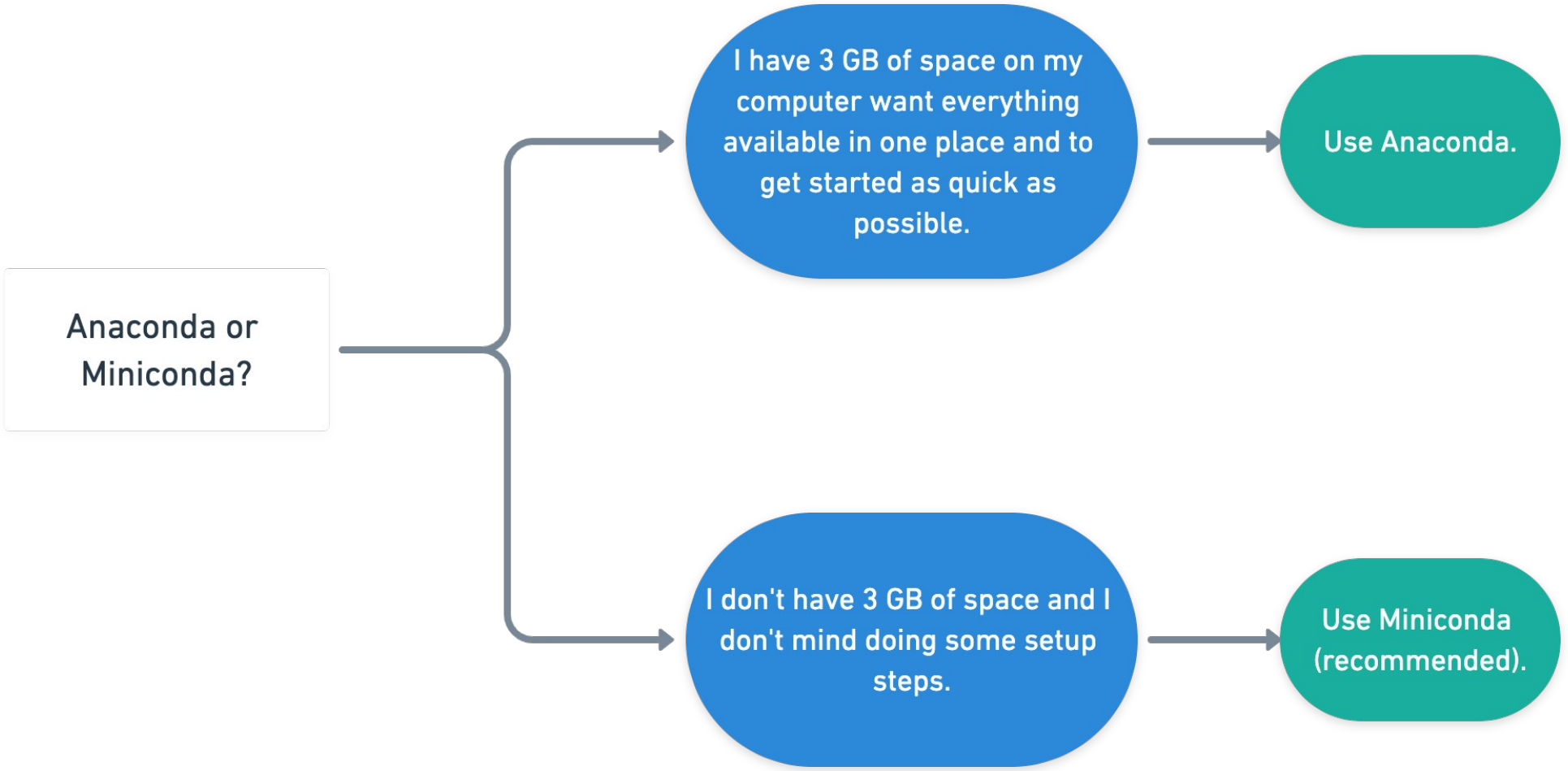
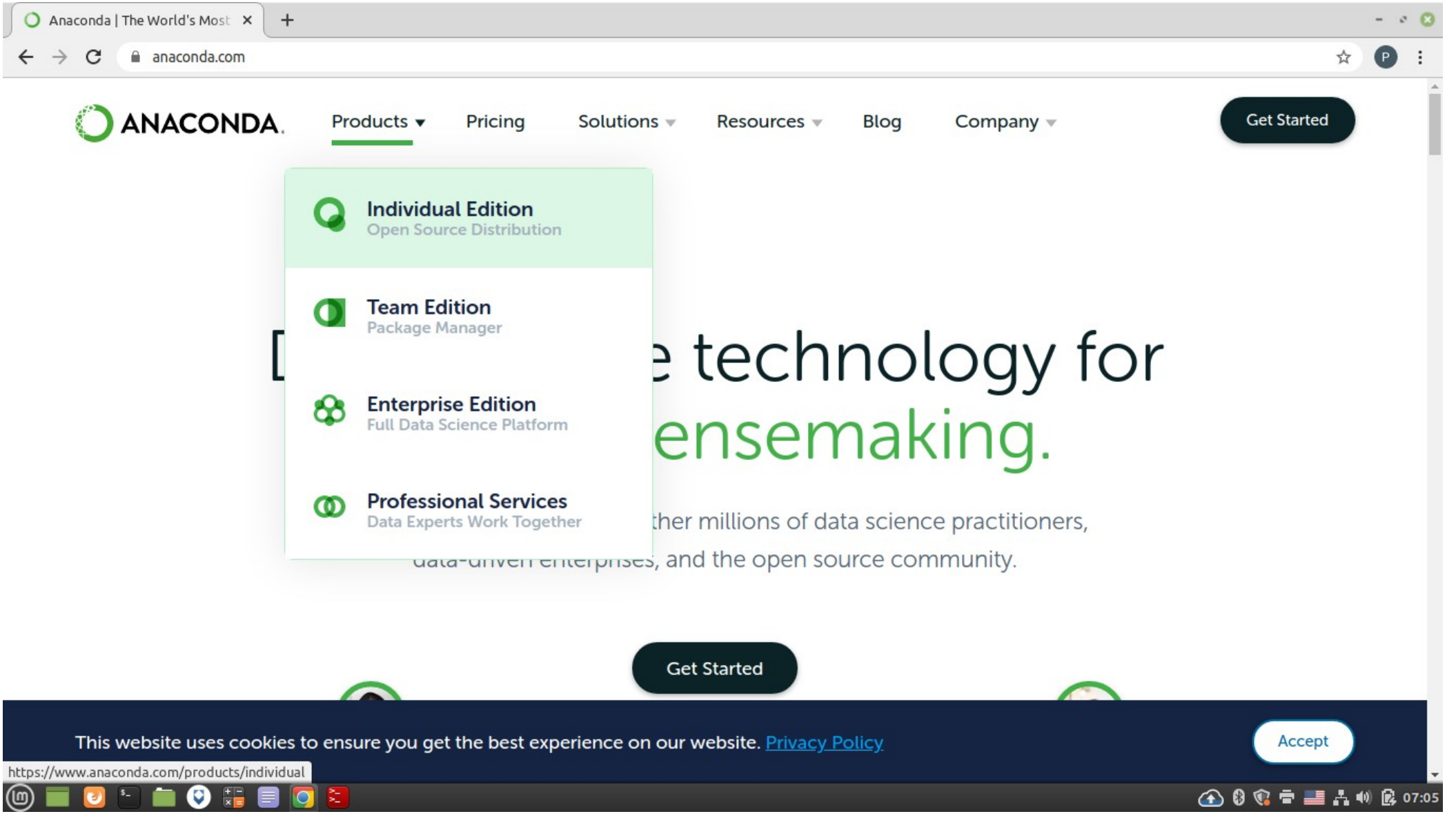


Installing Anaconda



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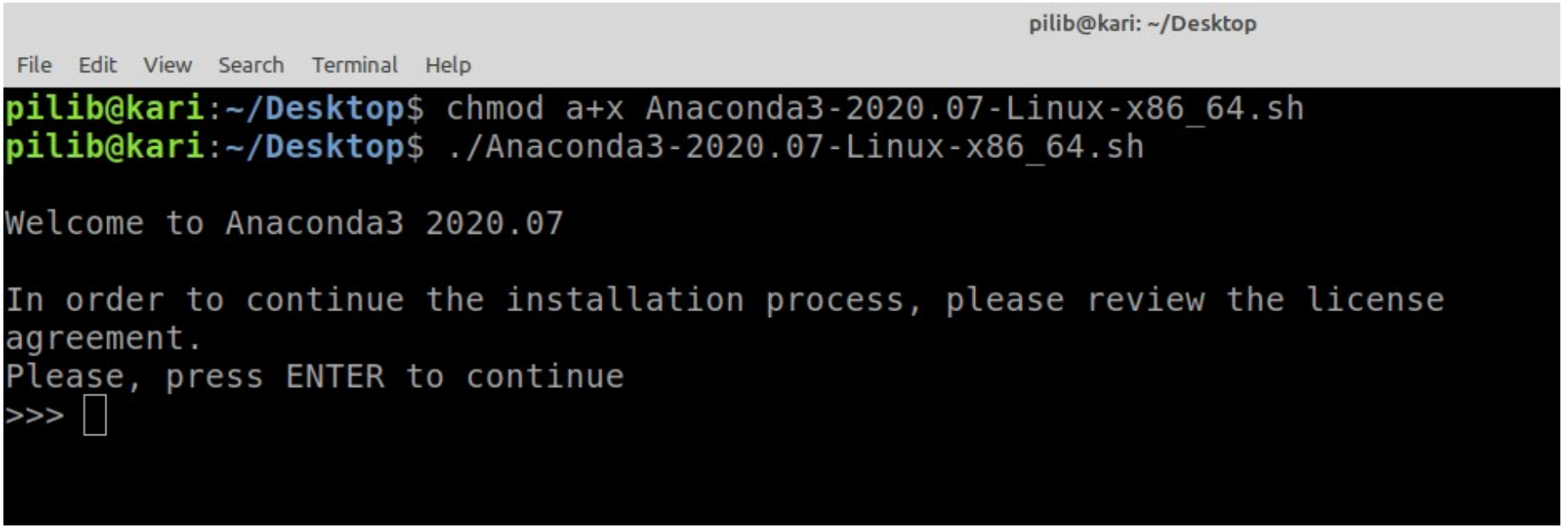
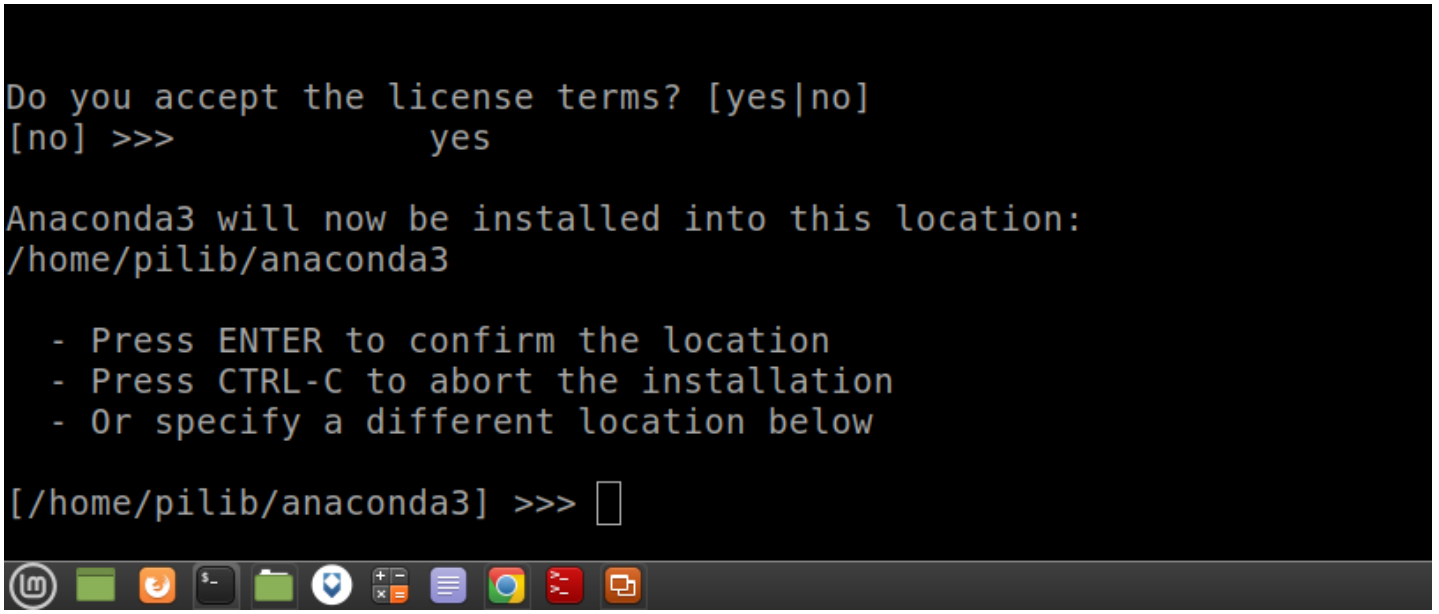




Installing Anaconda

```
  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
  wrapt                 pkgs/main/linux-64::wrapt-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
  xmltodict             pkgs/main/noarch::xmltodict-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-
                          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
```

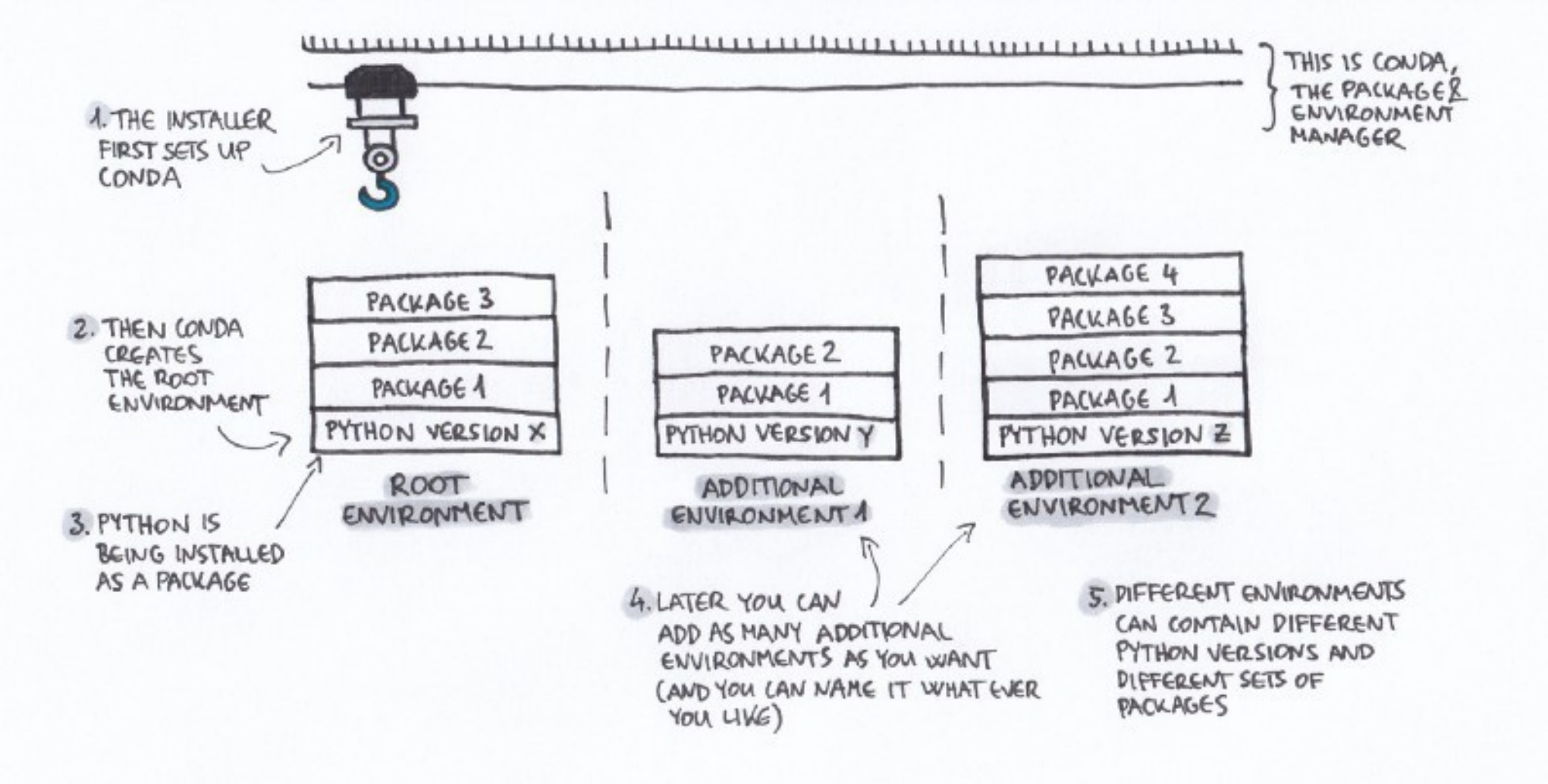
Updating Anaconda

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



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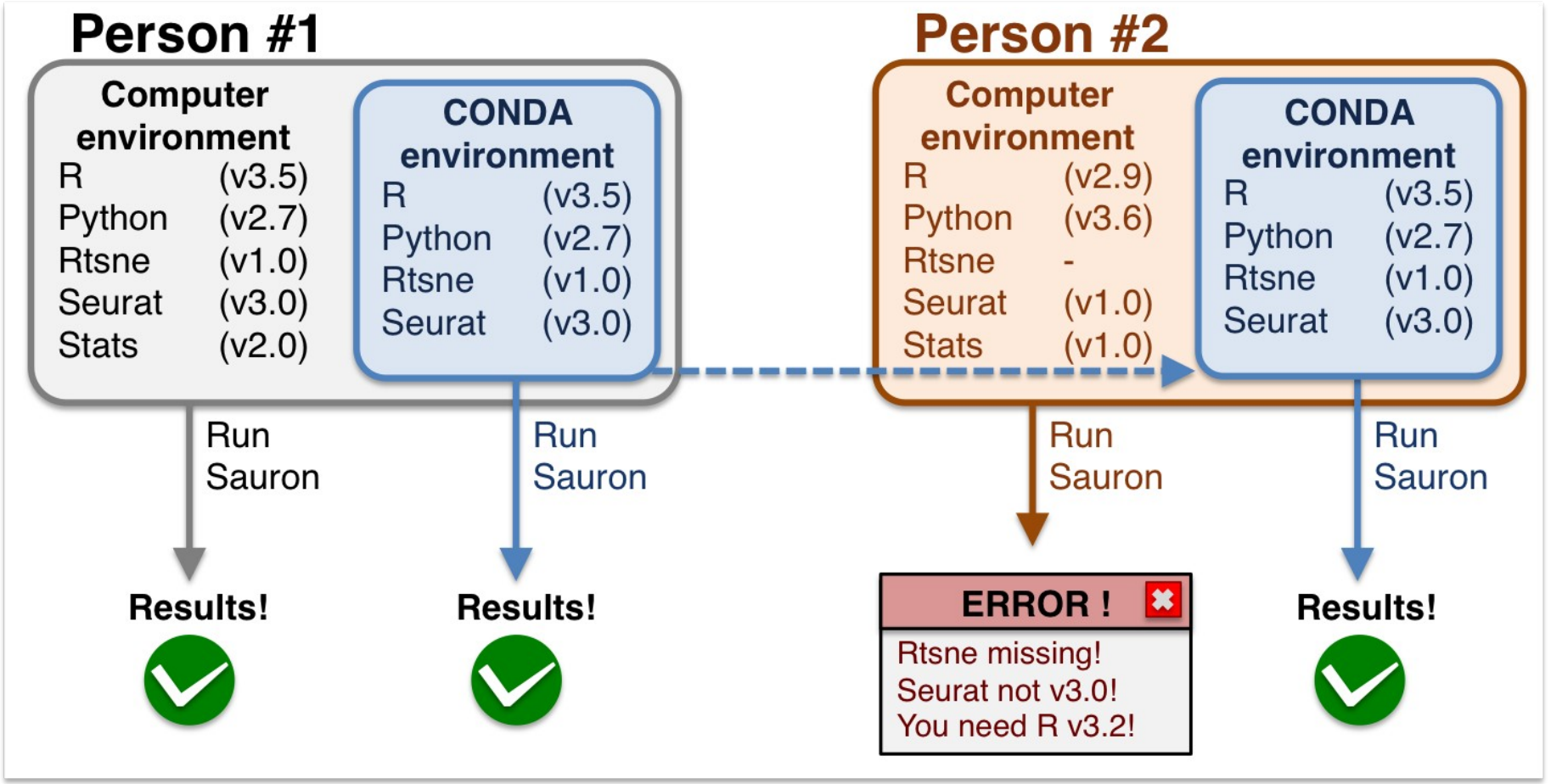


Managing Environments

conda env list # list all environments (* = current)

conda create -- name test # create new env called test

conda activate test # 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
```

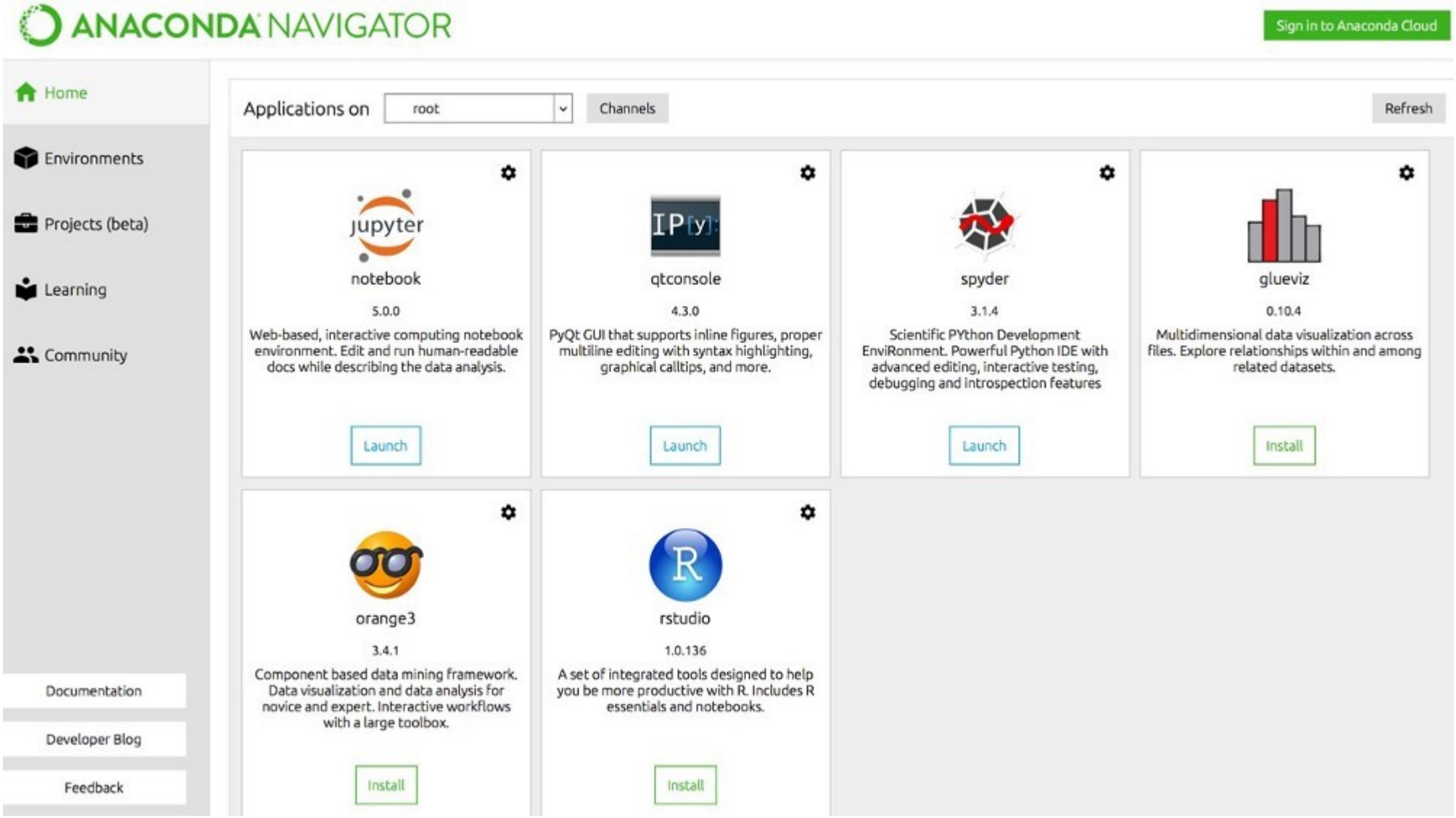
```
(test) pilib@kari:~$ python
Python 2.7.14 |Anaconda, Inc.| (default, Mar 27 2018, 17:29:31)
[GCC 7.2.0] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

Managing Channels

- Conda channels are repositories – collections of software

  conda config --add channels CHANNELNAME

  conda install CHANNELNAME::PKGNAME

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

Anaconda Navigator