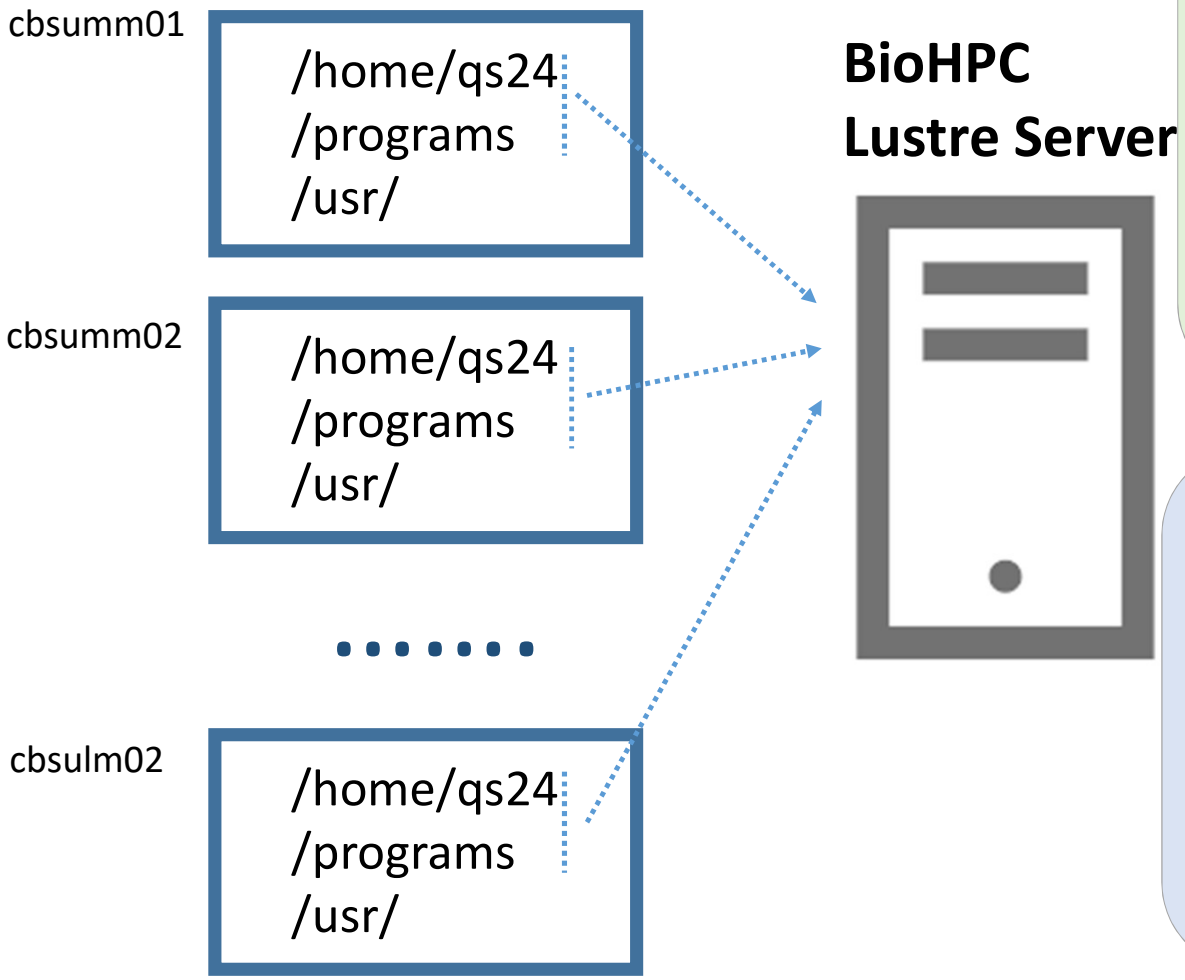
Software Locations on BioHPC



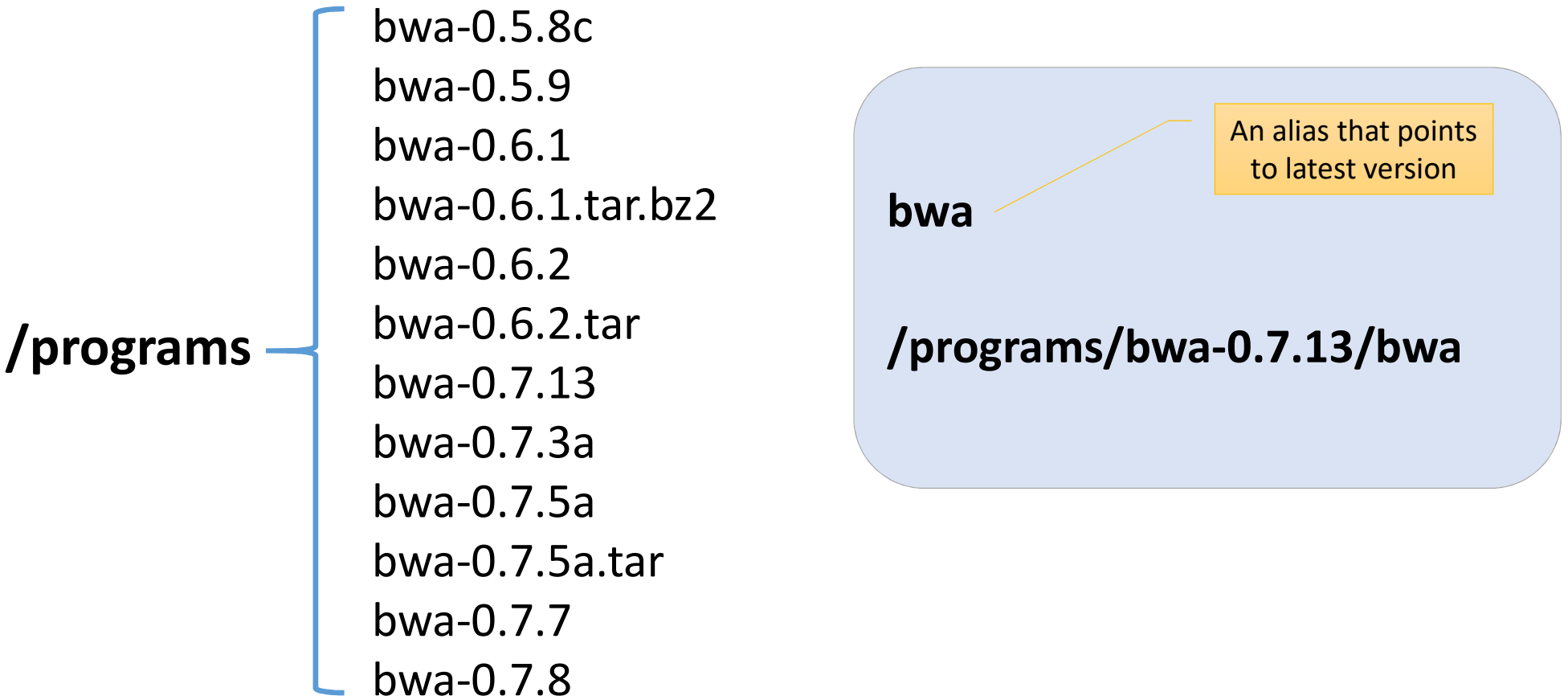
/usr or /usr/local

- Fast to load;
- Each computer might has different versions;

/programs

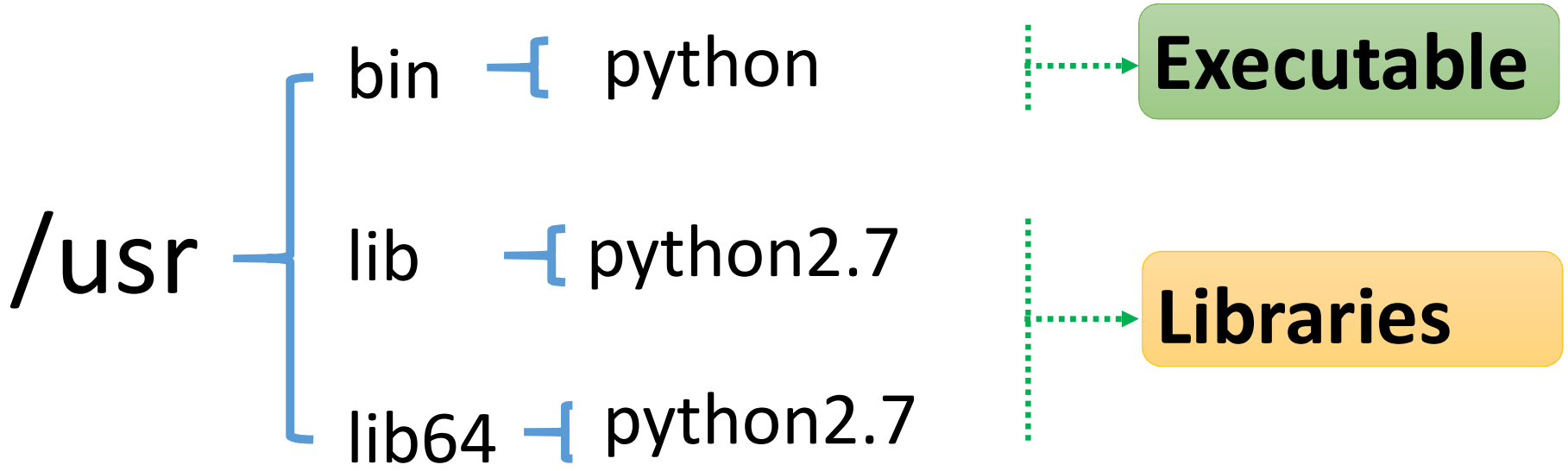
- A single copy is used by all machines;
- Slow to load;
- All versions kept;

All historic versions are kept in /programs/



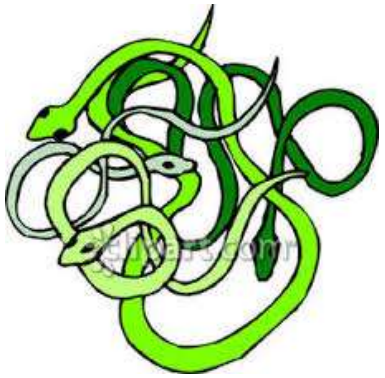
PYTHON

On a Brand New Server



PYTHON

After a while ….

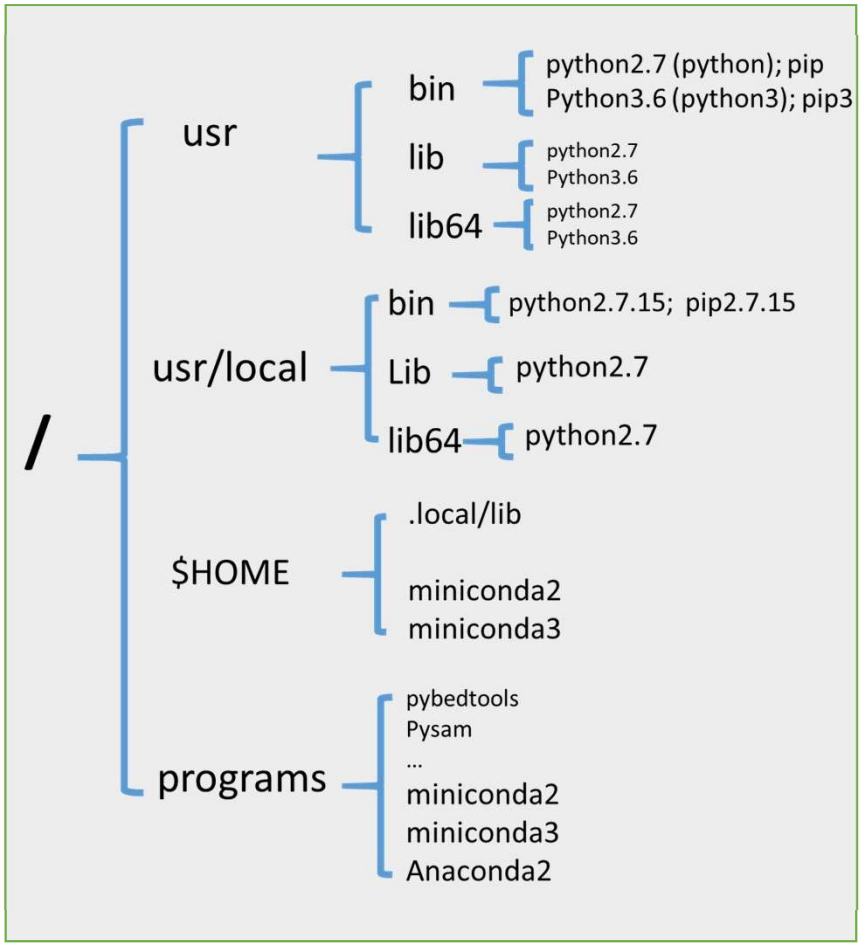


- /
  - usr
    - bin
      - python2.7 (python); pip
      - Python3.6 (python3); pip3
    - lib
      - python2.7
      - Python3.6
    - lib64
      - python2.7
      - Python3.6
  - usr/local
    - bin
      - python2.7.15; pip2.7.15
    - Lib
      - python2.7
    - lib64
      - python2.7
  - $HOME
    - .local/lib
    - miniconda2
    - miniconda3
  - programs
    - pybedtools
    - Pysam
    - …
    - miniconda2
    - miniconda3
    - Anaconda2

Instructions for Python on BioHPC

https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=556#c

PYTHON



Precedence

Executables

$PATH

- /usr/local/bin
- /usr/bin

Libraries

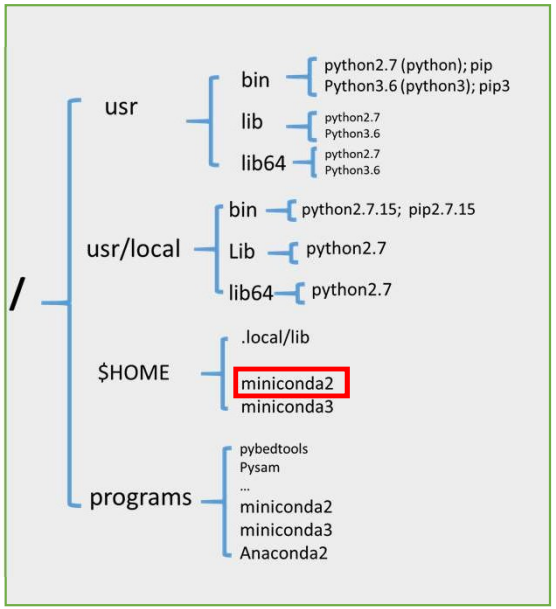
$PYTHONPATH

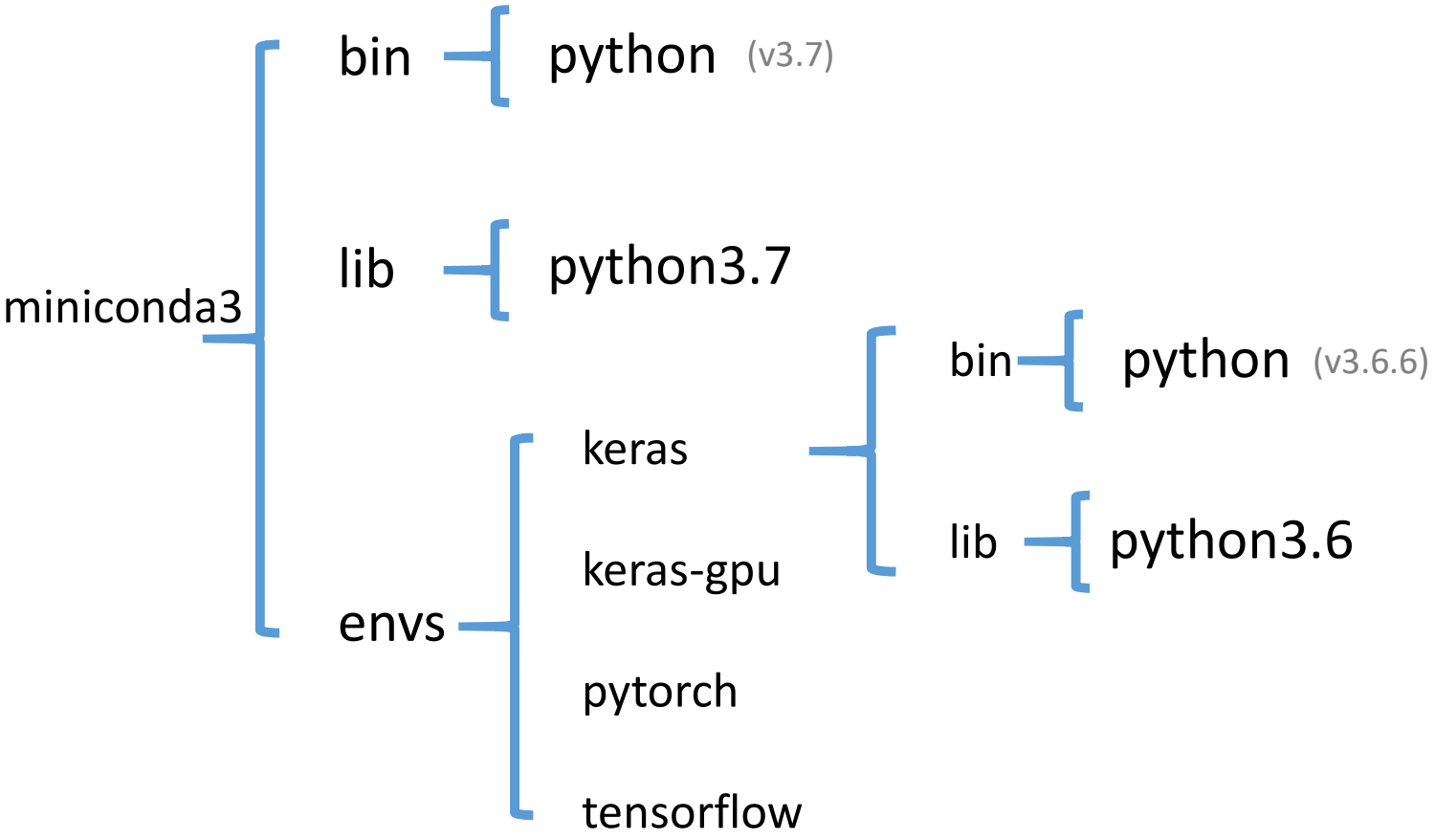
- sys.path (installation-dependent default)

- `export PATH=/programs/pybedtools/bin:$PATH`
- `export PYTHONPATH=/programs/pybedbools/lib64`
- `unset PYTHONPATH`

PYTHON

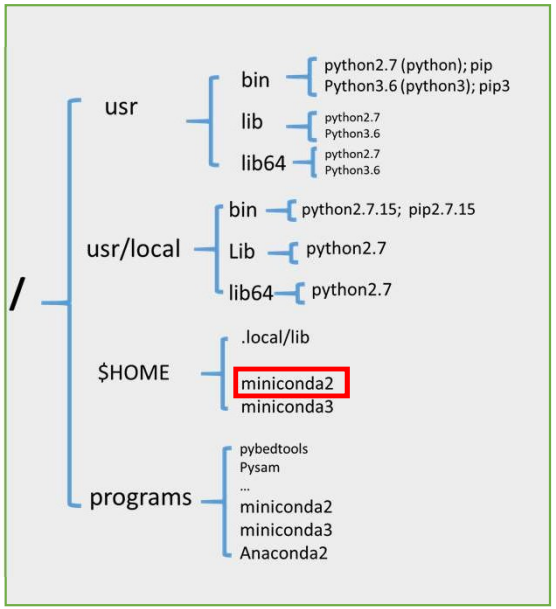
Using Conda

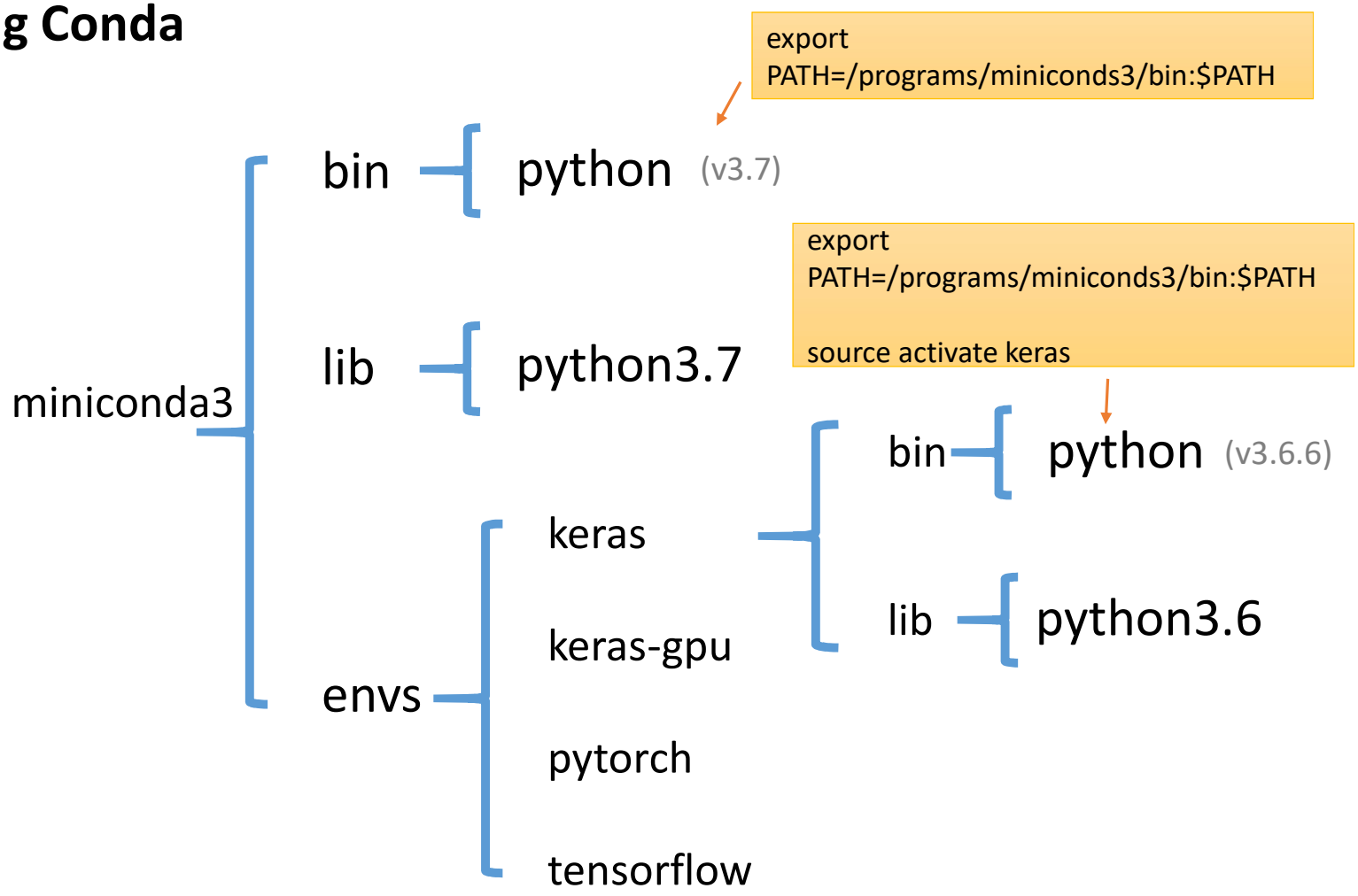


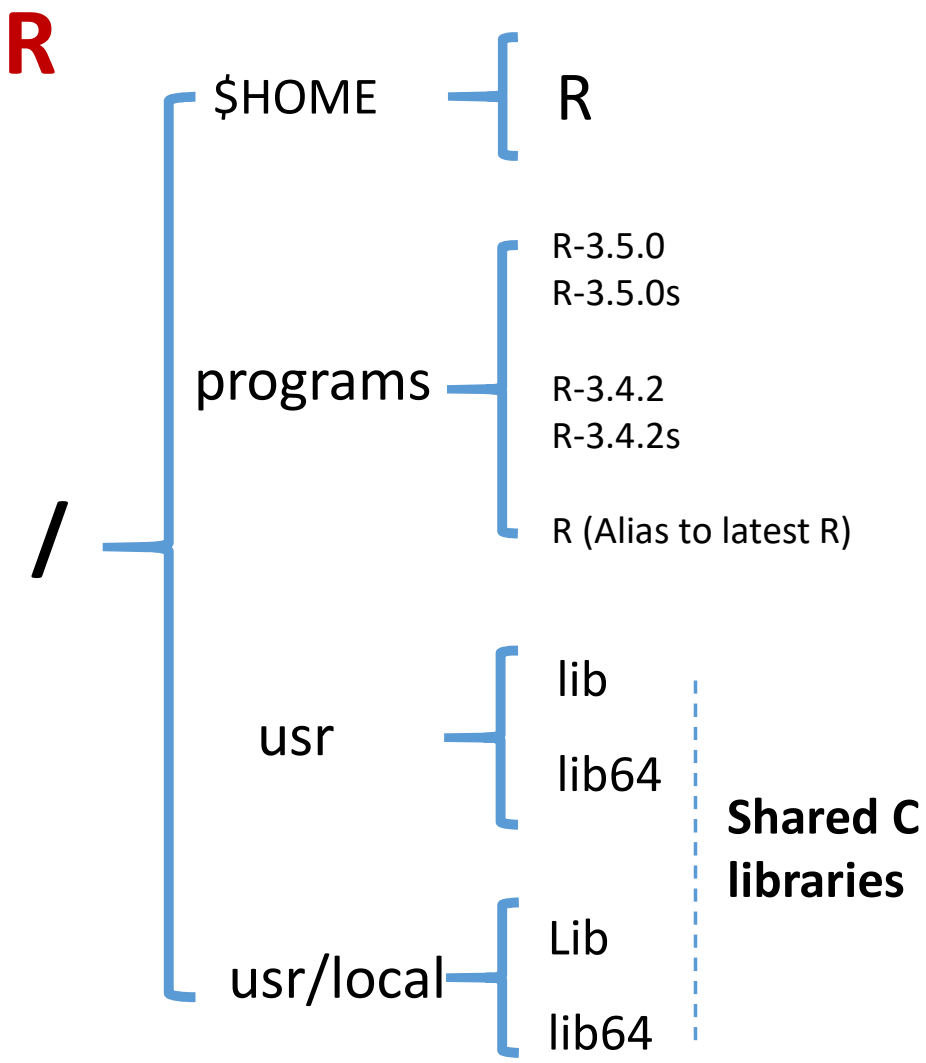


PYTHON

Using Conda







Note 1. Two separate installation for each version

R

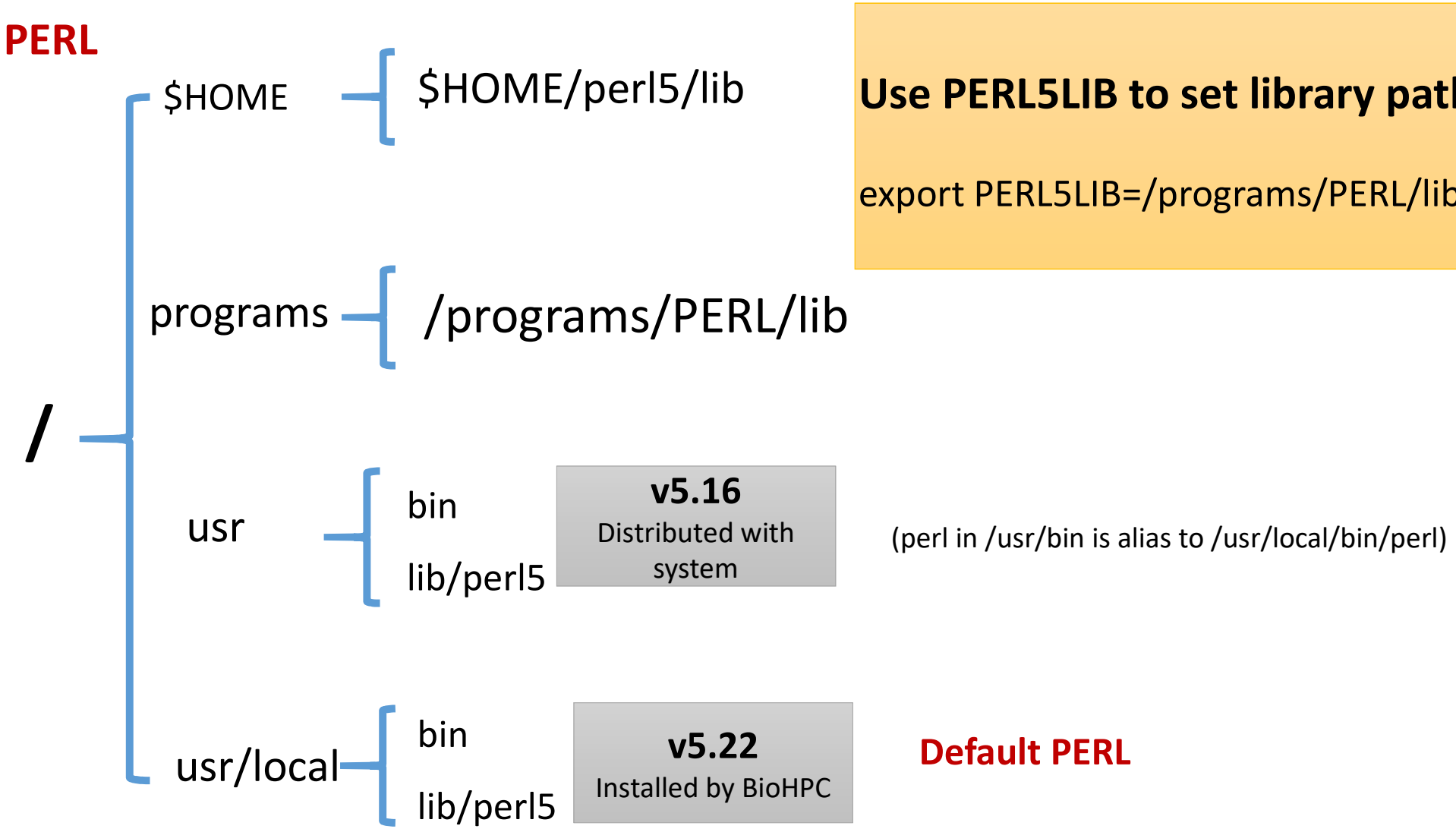
- Using parallel BLAS library
- Location: /programs/R/bin/R

/programs/R-3.5.0s/bin/R

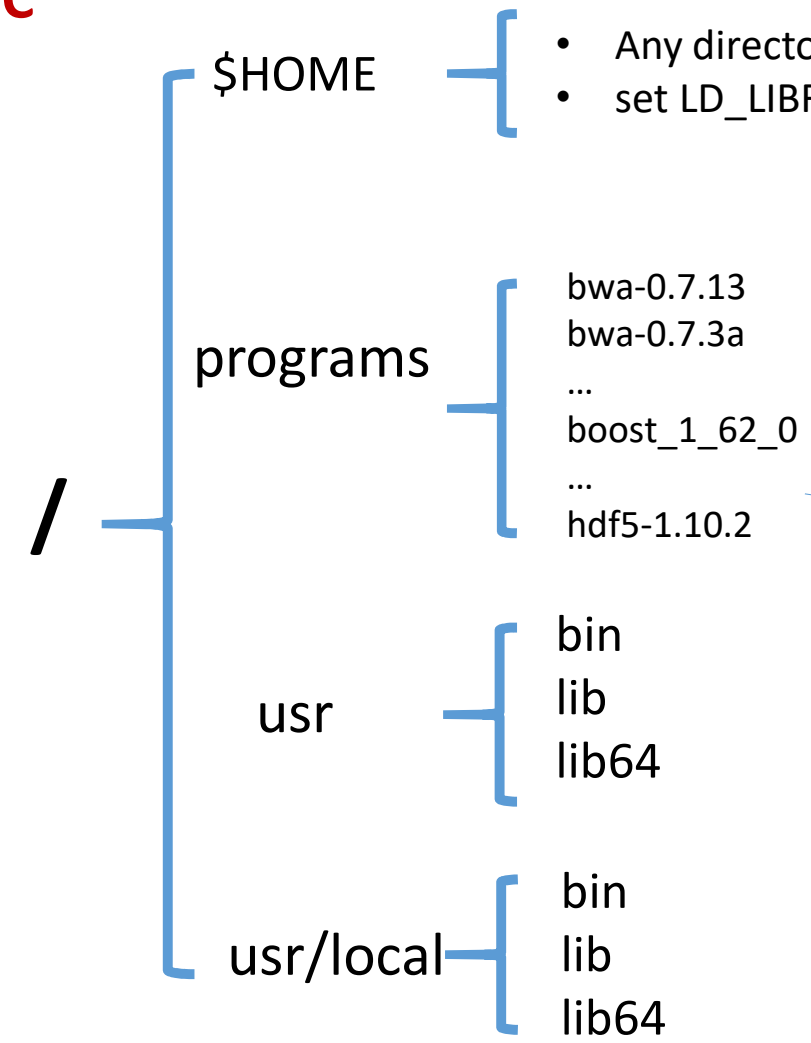
- Using built-in BLAS library

R in Conda Environment

Libraries in $HOME/R has precedence over conda environment.


PERL
/
$HOME
$HOME/perl5/lib
programs
/programs/PERL/lib
usr
bin
lib/perl5
v5.16
Distributed with system
usr/local
bin
lib/perl5
v5.22
Installed by BioHPC
Use PERL5LIB to set library path
export PERL5LIB=/programs/PERL/lib/perl5
(perl in /usr/bin is alias to /usr/local/bin/perl)
Default PERL

C



To use extra libraries:

export LD_LIBRARY_PATH=/programs/ hdf5-1.10.2/lib

C

Compiler

Default: /usr/bin/gcc (v.4.8.5)

Updated versions:

- /usr/local/gcc-5.5.0
- /usr/local/gcc-7.3.0

```
export LD_LIBRARY_PATH=/usr/local/gcc-7.3.0/lib:/usr/local/gcc-7.3.0/lib64

export PATH=/usr/local/gcc-7.3.0/bin:$PATH
```

C

CPU/GPU Types

	AVX	AVX2
General	X	X
Gen1 (Medium and Large mem.)	✓	X
Gen2 & Extra large.	✓	✓

Software compiled on one type of computers might not run on a different type.

What if something goes wrong?

Which executable?

```
which python
```

Which library?

```
echo $PYTHONPATH

echo $LD_LIBRARY_PATH

echo $PERL5LIB
```

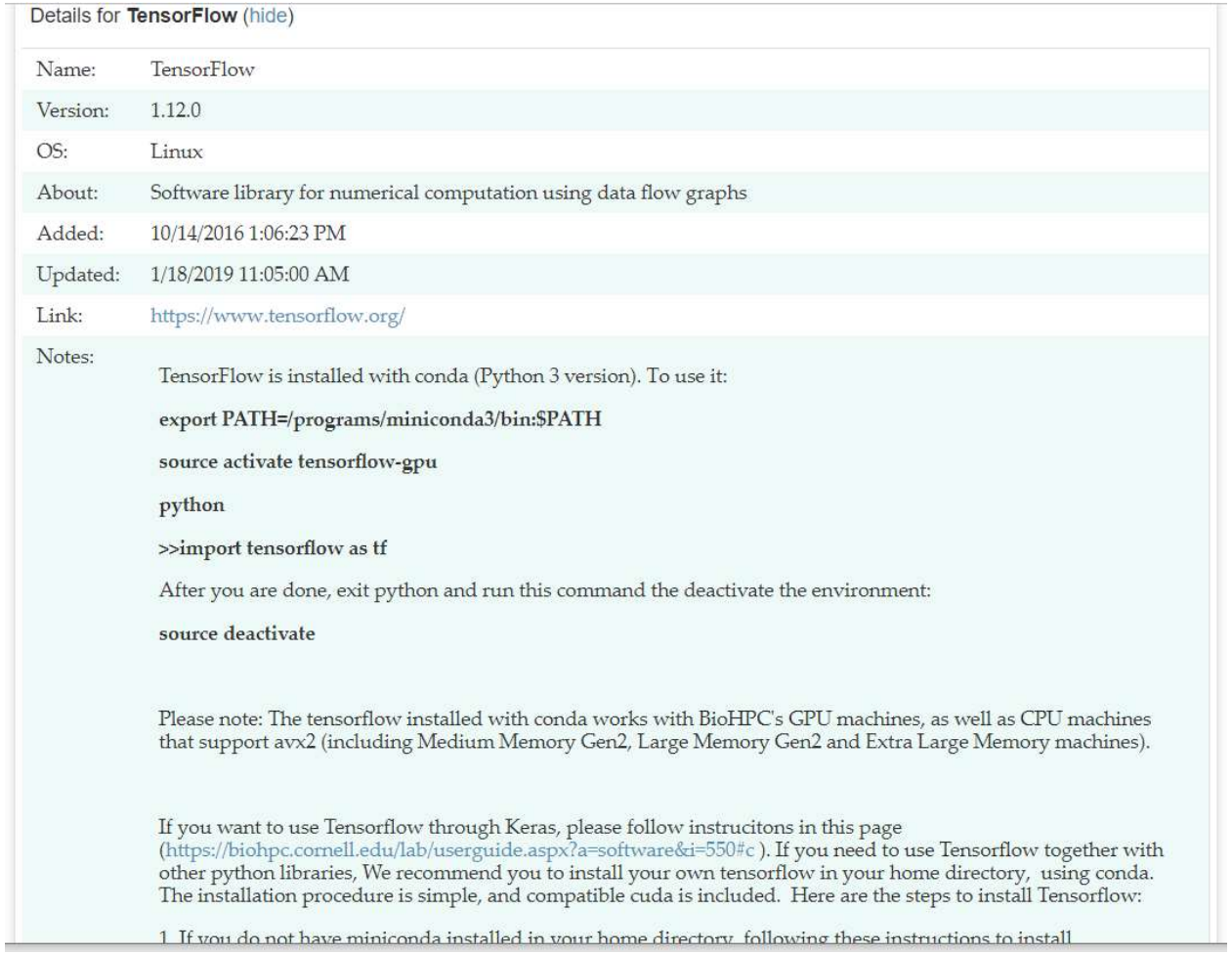
```
python
>import numpy
>numpy.__file__
```

```
C programs:
ldd /programs/bin/bwa/bwa
```

Check the .bashrc file

```
more $HOME/.bashrc
```

Software instruction page on BioHPC web site



Details for **TensorFlow** (hide)

Name:	TensorFlow
Version:	1.12.0
OS:	Linux
About:	Software library for numerical computation using data flow graphs
Added:	10/14/2016 1:06:23 PM
Updated:	1/18/2019 11:05:00 AM
Link:	https://www.tensorflow.org/
Notes:	TensorFlow is installed with conda (Python 3 version). To use it: **export PATH=/programs/miniconda3/bin:$PATH** **source activate tensorflow-gpu** **python** **>>import tensorflow as tf** After you are done, exit python and run this command the deactivate the environment: **source deactivate** Please note: The tensorflow installed with conda works with BioHPC's GPU machines, as well as CPU machines that support avx2 (including Medium Memory Gen2, Large Memory Gen2 and Extra Large Memory machines). If you want to use Tensorflow through Keras, please follow instrucitons in this page (https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=550#c). If you need to use Tensorflow together with other python libraries, We recommend you to install your own tensorflow in your home directory, using conda. The installation procedure is simple, and compatible cuda is included. Here are the steps to install Tensorflow: 1. If you do not have miniconda installed in your home directory, following these instructions to install

We do not support the "module" function to configure the shell.

Container and Software Installation Workshops

https://biohpc.cornell.edu/workshops.aspx