Software Locations on BioHPC

- **/usr or /usr/local**
  - Fast to load;
  - Each computer might have different versions;

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

```
cbsumm01
/home/qs24
/programs
/usr/

BioHPC Lustre Server
```
```
cbsumm02
/home/qs24
/programs
/usr/

/home/qs24
/programs
/usr/

......
```
```
cbsulm02
/home/qs24
/programs
/usr/
```
All historic versions are kept in /programs/

/programs

- bwa-0.5.8c
- bwa-0.5.9
- bwa-0.6.1
- bwa-0.6.1.tar.bz2
- bwa-0.6.2
- bwa-0.6.2.tar
- bwa-0.7.13
- bwa-0.7.3a
- bwa-0.7.5a
- bwa-0.7.5a.tar
- bwa-0.7.7
- bwa-0.7.8

/bwa

/programs/bwa-0.7.13/bwa

An alias that points to latest version
On a Brand New Server

/exec

Python

Executable

Libraries
PYTHON

After a while ....

Instructions for Python on BioHPC
https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=556#c
Precedence

**Executables**

- **$PATH**
  - `/usr/local/bin`
  - `/usr/bin`

**Libraries**

- **$PYTHONPATH**
  - `/programs/pybedtools/lib64`
  - `sys.path` (installation-dependent default)

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

```
/ 
usr 
lib 
lib64 
usr/local 
$HOME 
programs
```

```
bin: python2.7 (python); pip
  Python3.6 (python3); pip3
lib: python2.7
  python3.6
lib64: python2.7

bin: python2.7.15; pip2.7.15
lib: python2.7
lib64: python2.7

Local/lib

miniconda3

bin: python (v3.7)
lib: python3.7

envs

keras
keras-gpu
pytorch
tensorflow

bin: python (v3.6)
lib: python3.6
Using Conda

export PATH=/programs/miniconds3/bin:$PATH

source activate keras
Note 1. Two separate installation for each version

- 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.
Use PERL5LIB to set library path

export PERL5LIB=/programs/PERL/lib/perl5

Default PERL

perl in /usr/bin is alias to /usr/local/bin/perl

v5.16
Distributed with system

v5.22
Installed by BioHPC
To use extra libraries:

```
export LD_LIBRARY_PATH=/programs/ hdf5-1.10.2/lib
```
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
## CPU/GPU Types

<table>
<thead>
<tr>
<th></th>
<th>AVX</th>
<th>AVX2</th>
</tr>
</thead>
<tbody>
<tr>
<td>General</td>
<td>✗</td>
<td>✗</td>
</tr>
<tr>
<td><strong>Gen1</strong> (Medium and Large mem.)</td>
<td>✔</td>
<td>✗</td>
</tr>
<tr>
<td>Gen2 &amp; Extra large</td>
<td>✔</td>
<td>✔</td>
</tr>
</tbody>
</table>

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__`

### Check the `.bashrc` file
- `more $HOME/.bashrc`

### C programs:
- `ldd /programs/bin/bwa/bwa`
We do not support the “module” function to configure the shell.
Container and Software Installation Workshops

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

Please join our mailing list if you would like to be notified about new workshops.

Current Workshops
Introduction to BioHPC Cloud (February 4 and 6, 2019)
Linux for Biologists (February 11, 13, 18, 20, 25 and 27, 2019)
Practical Linux Examples in Bioinformatics (March 4 and 6, 2019)
Software installation on Linux (March 11, 13, 18 and 20 2019)
Using Docker in BioHPC Cloud (April 22 and 24 2019)