Georgia Advanced Computing Resource Center (GACRC) University of Georgia

http://www.gacrc.uga.edu/

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Overview

- Current status of software on zcluster (Sapelo)
- Application databases
- Installing by users
- Common problems/mistakes
- Troubleshoot
- Getting help from GACRC
Practice Script!

- Work at Interactive Node
  
  `cp -r /db/iprac .`
  
  `cd iprac`
  
  `less note.sh`
Installed Software

- GACRC Wiki Software page (zcluster, sapelo, version)  
  https://wiki.gacrc.uga.edu/wiki/Software

- Cluster onsite
  - Zcluster: `ls /usr/local/
  - Sapelo: `ls /usr/local/apps`

- Organized by package name

- Perl Python R packages
Application databases

- GACRC Wiki Software page (zcluster, sapelo, version)
  https://wiki.gacrc.uga.edu/wiki/Bioinformatics_Databases

- Cluster onsite

  
  ```
  ls /db/
  ls /db/ncbiblast
  ```
Obtain code – binary or source

Binary

- linux64
- Easy install
- May not compatible
- Slow performance

Source Code

- Need to compile
- Higher chance to be compatible
- Fast computing
Obtain code – get link

- Go to software website
- Getting major stable releases
- Getting tar.gz if available
- Getting source code if available

`wget http://...`
`curl -OL http://...`
Obtain code – get link (git)

```
git clone --recursive https://...
```

For bitbucket or google code
```
hg clone https://bitbucket.org/...
```
Decompress code package

- `gtar zxvf bamtools-1.0.2.tar.gz`
- `bunzip2 file.bz2`
- `unzip 10201_clusterware_linux32.zip`
- `tar xvf pygobject-3.19.2.tar`
Read manual

- Document on site:
  - README
  - INSTALL
  - doc/

- Document at website
Dependencies

- Check manual to meet requirement of Dependencies/ prerequisites
Compile and install

- `./configure`
- `make clean`
- `make`
- `make install`
Compile and install advanced

- ./configure --help
- ./configure
  --prefix=/home/rccstaff/yhuang/apps/hmmer-3.1b2
  > & 1 | tee yh.config.log
- make 2>&1 | tee yh.make.log
- make install 2>&1 | tee yh.install.log
Validating Installation

- Run test
- Run help

/home/rccstaff/yhuang/apps/hmmer-3.1b2/bin/hmmbuild -h
Perl and modules

- Perl version (v5.14.1)
- Test if perl lib `File::Basename` is installed
  ```perl
  perl -MFile::Basename -e 'print "Hello World\n"
  '"
  ```
- Add custom perl lib to PERL5LIB path:
  ```bash
  PERL5LIB=${PERL5LIB}:/usr/local/vcftools/latest/lib/perl5/site_perl
  ```
Install Perl Apps

- Script language, no need to compile
Python and Libraries

- Version
  - python2.7
  - python (python2.4)

- Test if python lib biom is installed
  python2.7 -c 'import biom; print biom.__file__'

- Add custom python lib to PYTHONPATH
  export PYTHONPATH=/usr/local/biom-format/1.1.2/lib/biom:${PYTHONPATH}
**Install Python Apps**

- `python2.7 setup.py build >&1 | tee yh.build.log`
- `python2.7 setup.py install --prefix=/home/rccstaff/yhuang/apps/cutadapt-1.9.1 >&1 | tee yh.install.log`
- **Validating**
  - `python2.7 /home/rccstaff/yhuang/apps/cutadapt-1.9.1/bin/cutadapt --help`
R and packages

- Default Version 3.0.3
- Test if package "phangorn" is installed
  \texttt{require("phangorn")}
Install R Package

- add package "phangorn" to user own lib

```r
install.packages("phangorn", repos="http://cran.r-project.org")
```
java

- Default Version 1.7.0_01
  ```
  java -version
  ```

- To use v1.8
  ```
  /usr/local/java/jdk1.8.0_05/bin/java -version
  ```

- To add classpath
  ```
  java -classpath 
  "/usr/local/bmge/latest/BMGE.jar" 
  Xms512m -Xmx1536m BMGE [options]
  ```
Support

- Submit ticket at GACRC support with detail of your command, dir of sample data, error message
- Submit requests with link of website, name and version of software