BioHPC: A High Performance Computing System for Life Sciences

Run/Install Software on BioHPC

Bioinformatics Facility
Biotechnology Resource Center
Cornell University
Software at BioHPC

- Many bioinformatics software packages pre-installed on BioHPC; new software can be installed on request
- See the BioHPC software webpage for instructions on how to run individual software title;
- Email brc_bioinformatics@cornell.edu if you would like software to be installed/updated;

Software Search Page:
https://biohpc.cornell.edu/lab/labsoftware.aspx

Instructions to Run Software

* We do not support module command to load software/pipeline.
To install software by yourself, we recommend setting up `Conda` environments in your home directory.

- **Anaconda for Python 2**
- **Miniconda for Python 2**
- **Anaconda for Python 3**
- **Miniconda for Python 3**

- Light, no extra libraries;
- Python 3 is more used now;
Where is software installed?

- On BioHPC servers, software installed in /programs;
- Software installed in /programs or your home directory are on network drive, and can be run from any BioHPC server except the login nodes.
How to run software?

• Most software are not in the default path. You need to check the instructions page before running software

BioHPC Software

bwa

or

/programs/bwa-0.7.8/bwa

User Installed Conda

Conda root:

export PATH=$HOME/miniconda2/bin:$PATH

bwa

Conda environment:

export PATH=$HOME/miniconda2/bin:$PATH

source activate bwa

bwa
Running software on BioHPC

• Use “screen” when running software;

• Parallelization of jobs:
  - perl_fork_univ.pl: perl_fork_univ.pl jobList 5
  - GNU parallel
  - Local scheduler (SLURM)
Supported containers:

Docker (a slightly restricted implementation for security)

https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=340#c

Singularity

https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=543#c
Other Software Related Information

(categorize by programming languages)
Some software require a specific version of library to compile.

Commonly used C libraries, including boost, HDF5 have multiple versions of libraries installed in /programs. Set LD_LIBRARY_PATH to use these libraries.

E.g. boost_1_46_1
     boost_1_55_0
     boost_1_57_0
     boost_1_58_0
     boost_1_62_0

Compilers:

Default: gcc v4.8.4

Alternative versions: 7.3.0, 5.5.0

To use alternative versions:

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

Libraries:
**PYTHON**

**Python commands:**
- `python` : python v2.7.5
- `python3` : python v3.6
- `python2.7.15` : python v2.7.15

(Corresponding pip commands: `pip`, `pip3`, `pip2.7.15`)

Updated python information can be found at:
[https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=556#c](https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=556#c)

**Jupyter Notebook:**
Implemented on each BioHPC server

To find more information about Jupyter Notebook on BioHPC, go to:
[https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=263#c](https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=263#c)
Commands:

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

```
/programs/R-3.5.0s/bin/R
```
- Using built-in BLAS library

R studio
Both "RStudio Server" and "RStudio Desktop" are implemented on BioHPC.

For updated R information, see this page:
https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=37#c

To find more information about R studio on BioHPC, go to:
https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=199#c
JAVA

Default Java version:

Java 8 (jdk1.8.0_121)

Update information can be found at:
https://biohpc.cornell.edu/lab/userguide.aspx?a=software&i=199#c

To use alternative versions

export JAVA_HOME=/usr/local/jdk1.7.0_51
export PATH=$JAVA_HOME/bin:$PATH
Use PERL5LIB to set library path

export PERL5LIB=/programs/PERL/lib/perl5

$HOME

$HOME/perl5/lib

programs

/usr

bin

lib/perl5

/usr/local

bin

lib/perl5

v5.16

Distributed with system

v5.22

Installed by BioHPC

Default PERL

BioHPC PERL modules

/perl5/lib

(perl in /usr/bin is alias to /usr/local/bin/perl)
Happy Computing!

The BioHPC Team

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