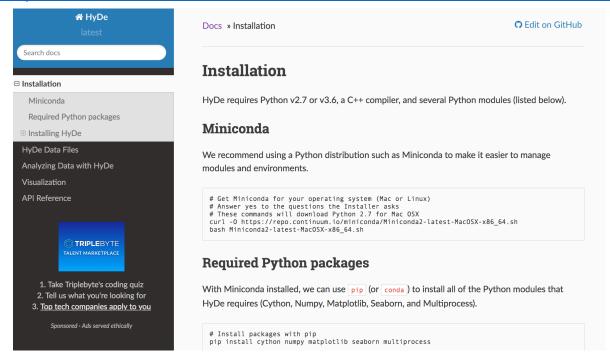
Python Package Install: miniconda

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Computational Biology Core



- Example:
 - HyDe install
 - https://hybridization-detection.readthedocs.io/installation.html



Start an interactive session using srun

\$ srun --mem=1G --partition=general --qos=general --pty bash

- Insalling Minicoda https://conda.io/docs/user-guide/install/linux.html
 - https://conda.io/miniconda.html

Miniconda

	Windows	Mac OS X	Linux
Python 3.7	64-bit (exe installer) 32-bit (exe installer)	64-bit (bash installer)	64-bit (bash installer) 32-bit (bash installer)
Python 2.7	64-bit (exe installer) 32-bit (exe installer)	64-bit (bash installer)	64-bit (bash installer) 32-bit (bash installer)

• wget https://repo.continuum.io/miniconda/Miniconda2-latest-Linux-x86_64.sh

Run the downloaded bash script using:

sh Miniconda2-latest-Linux-x86_64.sh

This will install miniconda in your home directory /home/FCAM/\$USER/miniconda2

Once installed it will add the miniconda path to your .bashrc file # added by Miniconda2 installer export PATH="/home/FCAM/\$USER/miniconda2/bin:\$PATH"

For this change to become active, you have to open a new terminal.

- Open a new terminal / interactive session
 - conda install will be active
- To test the conda is active type
 - > conda list

#			
# Name	Version	Build	Channel
asn1crypto	0.24.0	py27_0	
ca-certificates	2018.03.07	0	
certifi	2018.8.24	py27_1	
cffi	1.11.5	py27he75722e_1	
chardet	3.0.4	py27_1	
conda	4.5.11	py27_0	
conda-env	2.6.0	1	
cryptography	2.3.1	py27hc365091_0	
enum34	1.1.6	py27_1	
futures	3.2.0	py27_0	
idna	2.7	py27_0	
ipaddress	1.0.22	py27_0	
libedit	3.1.20170329	h6b74fdf_2	
libffi	3.2.1	hd88cf55_4	
libgcc-ng	8.2.0	hdf63c60_1	
libstdcxx-ng	8.2.0	hdf63c60_1	

- Update the conda
 - > conda update conda

- Install required packages for the program using conda
 - > conda install numpy

The following packages will be downloaded:

package	build	
mkl-2019.0	118	204.4 MB
numpy-1.15.3	py27h1d66e8a_0	36 KB
mkl_random-1.0.1	py27h4414c95_1	361 KB
numpy-base-1.15.3	py27h81de0dd_0	4.1 MB
blas-1.0	mkl	6 KB
mkl_fft-1.0.6	py27h7dd41cf_0	148 KB
intel-openmp-2019.0	118	721 KB
libgfortran-ng-7.3.0	hdf63c60_0	1.3 MB
	Total:	211.1 MB

The following NEW packages will be INSTALLED:

blas: 1.0-mkl
intel-openmp: 2019.0-118
libgfortran-ng: 7.3.0-hdf63c60_0
mkl: 2019.0-118
mkl_fft: 1.0.6-py27h7dd41cf_0
mkl_random: 1.01-py27h4414c95_1
numpy: 1.15.3-py27h1d66e8a_0
numpy-base: 1.15.3-py27h81de0dd_0

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Solving environment: failed

PackagesNotFoundError: The following packages are not available from current channels:

- multiprocess

Current channels:

- https://repo.anaconda.com/pkgs/main/linux-64
 https://repo.anaconda.com/pkgs/main/noarch
 https://repo.anaconda.com/pkgs/free/linux-64
 https://repo.anaconda.com/pkgs/free/noarch
 https://repo.anaconda.com/pkgs/r/linux-64
 https://repo.anaconda.com/pkgs/r/noarch
 https://repo.anaconda.com/pkgs/pro/linux-64
 https://repo.anaconda.com/pkgs/pro/noarch
- To search for alternate channels that may provide the co looking for, navigate to

https://anaconda.org

and use the search bar at the top of the page.

‡ Favorites	▼ Downloads	Package (owner / package)		Platforms
0	44012	O cvxgrp / multiprocess 0.70.4	conda	linux-64 osx-64 win-64
0	42762	oconda-forge / multiprocess 0.70.6.1 better multiprocessing and multithreading in python	conda	linux-64 osx-64 win-32 win-64
0	2378	omnia / multiprocess 0.70.4 better multiprocessing and multithreading in python	conda	linux-64 osx-64 win-32 win-64
				linux 64

> conda install -c conda-forge multiprocess

- Installing HyDe
 - > git clone https://github.com/pblischak/HyDe.git
 - > cd HyDe
 - > python setup.py install
 - Installed /home/FCAM/\$USER/miniconda2/lib/python2.7/site-packages/phyde-0.4.2-py2.7-linux-x86_64.egg
- Some times there might be version dependences
 - conda search -f cython
- To install a specific version
 - conda install cython==0.25

Xanadu Cluster Information

Understanding the Xanadu HPC Resource

- 1. What is a cluster
- 2. How to obtain an account
- 3. How to reset a password
- 4. How to access the Xanadu cluster
- 5. HPC resources and limits
- 6. Working with Slurm (Running interactive jobs and submission scripts)
- Resource Limitations
- 2. Different ways of Running Jobs
- 3. How to submit, Monitor and Cancel a Job
- 7. How to load software
- 8. File system
- 9. How to Transfer Data Between Clusters

What is a cluster

A desktop or a laptop, in most cases, is inadequate for analysis of large scale datasets (e.g. Genomics) or to run simulations (e.g. protein docking). They lack both the processing power and the memory to execute these analyses. This limitation can be overcome by combining machines (computers) in a predefined architecture/configuration so that they act as a single unit with enhanced computational power and shared resources. This is the basic concept of a high performance cluster. A cluster consists of a set connected computers that work together so that they can be viewed as a single system. Each computer unit in a cluster is referred as 'node'.

The components of a cluster are usually connected through fast local area networks ("LAN"), with each node running its own instance of an operating system. The benefits of clusters include low cost, elasticity and the ability to run jobs anytime. anywhere.

Install Python and R packages in local (home) directories

This short tutorial will provide instruction for installing and loading Python and R packages in your home directory without administrative access. We will use alfpy, remeta and ggplot2 in this tutorial.

Install python package alfpy via pip

Pip is a package management system used to install/manage software packages from Python Package Index. Pip is simple and user friendly. Usually, as users, we don't need to worry about prerequisites when we install a package via pip. Since pip has already been globally installed in BBC/Xanadu, and alfpy can be found in Python Package Index, we can use the following command from the home directory (the first location you arrive at after login to BBC or Xanadu).

pip install --user alfpy

note that flag —user is required because pip by default will install packages in root packages directory where most of users do not have permission to make changes.

Sometimes the latest version of a package is not compatible with the latest Python version in BBC/Xanadu or some features you need only exist in a certain version. Try to install an older version if you encounter this issue. To install alfpy 1.0.4. we first need to make sure current version of the package is uninstalled (note that flag "–user" is not required to uninstall).

pip uninstall alfpy

Then begin installation by entering:

https://bioinformatics.uconn.edu/resources-and-events/tutorials/