Using Conda on the GACRC Sapelo2 Cluster


• CONDA has come out on top in some ways and is becoming a popular choice for scientific software deployment

• In intention it is similar to language packaging systems, such as Python pip with virtualenv and Rubygems with bundler, but its scope is wider because it includes a build environment

• CONDA itself builds on top of the underlying software distribution using C compilers and such. In addition it manages a subset of low level libraries (including readline, ncurses, libxml2). It rather is a distribution in a distribution that can act fully in user land and provides source and binary deployment.
1. The installer first sets up Conda

2. Then Conda creates the root environment

3. Python is being installed as a package

4. Later you can add as many additional environments as you want (and you can name it whatever you like)

5. Different environments can contain different Python versions and different sets of packages
A simple example on Sapelo2

1. qlogin (open an interactive session for building your conda environment)
2. ml Miniconda3/4.4.10-refresh (load Miniconda3 fresh version)
3. mkdir ./myenv (the full path to env location will be /home/username/myenv)
4. conda create -p /home/username/myenv/ (create your own env at the location created in step 3)
5. conda env list
6. source activate /home/username/myenv
7. conda list
8. conda install numpy==1.16.2 (install numpy/1.16.2) (conda uninstall/remove)
9. conda install matplotlib (install latest matplotlib)
10. python program.py (run your python script in your conda virtual env)
11. conda deactivate (conda env list)
12. conda remove /home/username/myenv
A practical example on Sapelo2

1. `qlogin` (open an interactive session for building your conda environment)
2. `ml Miniconda3/4.4.10-fresh` (load Miniconda3 fresh version)
3. `mkdir ./env-busco` (the full path to env location will be `/home/username/env-busco/`)
4. `conda create -p /home/username/env-busco/` (create the env at the location created in step 3)
5. `conda env list`
6. `source activate /home/username/env-busco`
7. `conda install -c bioconda busco` (install busco env via additional channel, e.g. bioconda, conda-forge)
8. `python /home/username/env-busco/bin/run_BUSCO.py -h` (run busco help info)
Conda cheat sheet is at


https://kapeli.com/cheat_sheets/Conda.docset/Contents/Resources/Documents/index