Working with Anaconda/Miniconda

What is Anaconda?

Anaconda is a distribution platform and toolkit for running independent software environments, especially for python but it can be used for almost any software component. So if you need a specific version of python, or a specific version of some of its modules, this may be the place to go. Anaconda is a full environment, Miniconda is the minimal set to get started. Both will function the same once installed and configured

See Anaconda website for more information and downloads

Installing Anaconda

Method 1: Download and install

You can install anaconda or Miniconda (see anaconda website). This downloads a shell script you can run (either chmod 755 to make it executable, or run 'bash Miniconda3-latest-Linux-x86_64.sh' or whatever the name of your download is. Choose the location where you want to install the distribution (in a directory you own, but if you plan to install a lot of software, you should probably not install it in your home directory).

Method 2: Use EasyBuild installed versions of Miniconda

We have pre-installed versions of Miniconda available through EasyBuild. Run

module load Miniconda3

to load it (or check first using module avail Miniconda what versions are available. You will see that there may also be Miniconda environments with some software already installed.

Setup

Now that you have the conda package manager available, you can use it to complete the setup.

Creating an environment

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Installing packages

Pitfalls

As you can see above, the default behaviour when installing conda or running conda init is, to add some code to your .bashrc or .tcshrc to activate conda on every shell and in every window you open. That may sound like a nice feature, until you realize, that a custom version of python with a custom set of packages may wreak havoc on any environment that relies on the system default version. And there is a lot of software that happens to be written in python, or linked with it, including big parts of the Gnome and Cinnamon desktop applications. So, if you happen to set up a non-standard version of python as default, it might not be possible for you to log in in these desktop environments any more. Or even worse, if you need to install non-standard versions of gcc or its libraries, you might not be able to run a big part of the system software any more.

Solutions to these pitfalls

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