

Using Conda and Anaconda

Conda is a package manager system for Python and other tools and is widely used in some areas such as bioinformatics and data science. On personal computers it is a useful way to install a stack of tools.

The full documentation can be found at

<https://docs.conda.io/projects/conda/en/latest/user-guide/index.html>

Warning: Conda, whilst convenient, is not designed to be installed on multi-user compute clusters and we are unable to guarantee that tools installed via it will work correctly. This is especially true for any parallel (MPI) tools.

Setting up Conda

First load the appropriate modules

```
$ module load gcc miniconda3
```

And the first time you use it

```
$ conda init bash
```

This command will hang on a sudo password input, just ignore it (ctrl-c)

You will now probably need to log out and back in again to "activate" the changes.

Once you log in again conda should be available.

Please ignore any messages about updating to a newer version of conda!

Configuring Conda

By default Conda will put everything including downloads in your home directory. Due to the limited space available this is probably not what you want.

We strongly recommend that you create a `.condarc` file in your home directory with the following options:

```
pkgs_dirs:  
- /work//path/to/my/project/space
```

where the path is the path to your project space on /work - we do not recommend installing things in /scratch as they might be automatically deleted.

You may also wish to add a non standard `env_dirs`

```
envs_dirs:  
- ~/myproject-envs
```

Please see the full `condarc` documentation for all the possible configuration options

<https://docs.conda.io/projects/conda/en/latest/user-guide/configuration/use-condarc.html>

Using Conda virtual environments

The basic commands for creating conda environments are:

Creation

```
$ conda create --name $MY_CONDA_ENV_NAME
```

Activation

```
$ conda activate $MY_CONDA_ENV_NAME
```

Deactivation

```
$ conda deactivate
```

Environment in specific location

If you need to create an environment in a non standard location:

```
$ conda create --prefix $MY_CONDA_ENV_PATH
```

```
$ conda activate $MY_CONDA_ENV_PATH
```

```
$ conda deactivate
```

Installing packages

The base commands are:

```
$ conda search $PACKAGE_NAME
```

```
$ conda install $PACKAGE_NAME
```

Running Slurm jobs with conda

Since Conda needs some initialization before being used, a Sbatch script must explicitly ask to run bash in *login* mode. This can be performed by adding `--login` option to the shebang. Here is an example of Sbatch script using Conda:

```
#!/bin/bash --login

#SBATCH --time 00-00:05:00
#SBATCH --nodes 1
#SBATCH --ntasks 1
#SBATCH --cpus-per-task 1
#SBATCH --mem 4G

module load gcc miniconda3
conda activate $MY_CONDA_ENV_PATH

...
```

Revision #7

Created 23 July 2020 05:27:31 by Ewan Roche

Updated 20 May 2021 06:48:52 by Emmanuel Jeanvoine