

# 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 can be used freely for research purposes but pay attention to never use the "default" channel since it is not free in a research context like UNIL (<https://www.anaconda.com/blog/is-conda-free>). As a replacement to "default" channel, please use "conda-forge". If you have any doubt about that please contact us at [helpdesk@unil.ch](mailto:helpdesk@unil.ch) (and start the subject with DCSR).**

## Setting up Conda

First load the appropriate modules

```
dcsrsoft use 20241118  
module load miniforge3  
conda_init
```

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/conda_pkgs
```

```
auto_activate_base: false  
channels:  
  - conda-forge
```

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 --cpus-per-task 1
#SBATCH --mem 4G

dcsrsoft use 20241118
module load miniforge3
conda_init
conda activate $MY_CONDA_ENV_PATH

...
```

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