

Conda

Conda ist ein Paketmanager um reproduzierbar Software-Umgebungen auf Systemen zu installieren. Dabei werden Abhängigkeiten zu Bibliotheken automatisch aufgelöst und in vorkompilierter Fassung installiert.

Dies hat den Vorteil, dass man immer genau die gleiche Version einer Software installiert, egal auf welchem System man ist. Der Nachteil ist jedoch, dass oftmals keine Optimierungen für den konkret vorhandenen CPU berücksichtigt werden. Dies führt zu einer höheren Laufzeit der Programme.



Latest Information

Currently we have a mirror for Conda to allow you to install packages without internet access. You should specify these local mirrors, when you want to create a new environment

```
conda create -c http://conda.repo.test.hhu.de/bioconda -c http://conda.repo.test.hhu.de/main -c
http://conda.repo.test.hhu.de/conda-forge --override-channels --name my_environment
```

but also if you want to install new packages

```
conda install -c http://conda.repo.test.hhu.de/bioconda -c http://conda.repo.test.hhu.de/main -c
http://conda.repo.test.hhu.de/conda-forge --override-channels $PACKAGE_NAME
```

```
name: Example
channels:
  - nodefaults
  - http://conda.repo.test.hhu.de/bioconda
  - http://conda.repo.test.hhu.de/main
  - http://conda.repo.test.hhu.de/conda-forge

dependencies:
  - bwa = 0.7.17
  - samtools = 1.10
  - bcftools = 1.10.2
```

.condarc

To make your life super easy and just ignore all of the above (and thus also keep your existing .yaml files) you can also just create a .condarc file in your home directory with the following contents (this handles the redirection of the channels to the custom hhu ones for you):

```
channel_alias: http://conda.repo.test.hhu.de/

default_channels:
  - http://conda.repo.test.hhu.de/main
  - http://conda.repo.test.hhu.de/bioconda
  - http://conda.repo.test.hhu.de/conda-forge
```



modules

There are currently five different conda modules.

For normal usage utilize Miniconda/3. If you want to use conda within snakemake or have other specific needs you can try Miniconda/3_noInit or Miniconda/3_snakemake.

Miniconda/3.1 uses a newer version of Python (3.10.8) and pip.



Hinweis

If activating your conda environment works for you in interactive mode but not in batch mode, then you might need to source your files `.bashrc` and `.bash_profile`. This is because in interactive mode you'll get a login shell but in batch mode not. In your jobscript such a solution could look as follows:

```
#!/bin/bash
#PBS -l select=1:ncpus=X:mem=XGB
#PBS -l walltime=X:00:00
#PBS -A 'XXX'

# source bash
source $HOME/.bashrc
source $HOME/.bash_profile
conda activate SOME_ENV
```