Conda

Another example of **conda** environment setup.

Login on the submit node

Login on the cluster submission node, check the page *How to Access* for more information:

```
$ ssh -l <username> cirrus.ncg.ingrid.pt
[username@cirrus ~]$ _
```

Prepare a conda virtual environment

The default **python** version for *CentOS 7.x* is **2.7.5** which is not suitable for many applications. So, we will create a **python** virtual environment:

```
[username@cirrus ~]$ conda create -n myconda python=3.6
[username@cirrus ~]$ conda activate myconda
```

On the first command, where we create the **conda** virtual environment, you can include a list of applications to include on your environmnet, for example:

```
[username@cirrus ~]$ conda create -n myconda python=3.6 ipython-notebook numpy=1.6
```

Manage the conda virtual environment

It is possible to include additional packages to your **conda** environment, for example:

```
[username@cirrus ~]$ conda activate myconda
[username@cirrus ~]$ conda install numpy
```

You can update your software bandle on the **conda** virtual environment with the command:

```
[username@cirrus ~]$ conda update [scipy ...]
```

or remove a specific application:

```
[username@cirrus ~]$ conda uninstall tensorflow-gpu
```

Check the **conda** help for more information:

```
[username@cirrus ~]$ conda help
[username@cirrus ~]$ conda install --help
```

Manage the conda packages list with pip

It is possible to complemment the **conda** virtual environment packages list with **pip**. For example:

```
[username@cirrus ~]$ conda activate myconda
[username@cirrus ~]$ pip install --upgrade pip
[username@cirrus ~]$ pip install --upgrade setuptools
[username@cirrus ~]$ pip install tensorflow-gpu
[username@cirrus ~]$ pip install keras
```

Manage packages versions

If the applications available on **conda** virtual environment do not match your version requirements you may need to use packages from **pip** repostory; check the availability of *conda search* and *pip search* command line interfaces.

As an example we have the **tensorflow-gpu** package, when used with **keras**, the **conda** repository downgrades ***tensorflow-gpu** to version *1.15*, but you most likely will prefer version *2.0*. The **pip** repository has the right combination of **tensorflow-gpu** and **keras** packages.

We advise the user to install a package from only one repository in order to guarantee perfect behaviour.

Load conda environment on a batch job

Create a submit script:

```
[username@cirrus ~]$ cat submit.sh


#!/bin/bash


#SBATCH --job-name=MyFirstSlurmJob
#SBATCH --time=0:10:0
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=16


# Be sure to request the correct partition to avoid the job to be held in the queue, furthermore
# on CIRRUS-B (Minho)  choose for example HPC_4_Days
# on CIRRUS-A (Lisbon) choose for example hpc
#SBATCH --partition=HPC_4_Days
```

```
# check python version
python --version


# Load conda environment
conda activate myconda


# recheck python version
python --version


# your job payload
#....
```

Submit:

```
[username@cirrus ~]$ sbatch submit.sh
Your job 2037792 ("submit.sh") has been submitted
```

After completion:

```
[username@hpc7 ~]$ ls -l
-rwxr-----+ 1 username hpc   668 Jan  7 12:19 submit.sh
-rw-r-----+ 1 username hpc    44 Jan  7 12:18 submit.sh.e2037792
-rw-r-----+ 1 username hpc     0 Jan  7 12:18 submit.sh.o2037792


[username@cirrus ~]$ cat submit.sh.e2037792
Python 2.7.5
Python 3.6.9 :: Anaconda, Inc.
```

Some References

- [GitHub OS-agnostic](#)
- [Anaconda Documentation](#)
- [Conda Documentation](#)

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