How to Create Conda Environment in HPC

Login to HPC

Set proxy environment variables

- ***export http_proxy="http://10.8.0.1:8080"***
- ***export https_proxy="https://10.8.0.1:8080"***

Either run following commands or refer to the **documentation**

- ***mkdir -p ~/miniconda3***
- ***wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh -O ~/miniconda3/miniconda.sh***
- ***bash ~/miniconda3/miniconda.sh -b -u -p ~/miniconda3***
- ***rm -rf ~/miniconda3/miniconda.sh***
- ***~/miniconda3/bin/conda init bash***

After exiting and logging back into the HPC, you will now notice the '(base)' indicator at the command prompt.

Now create and open **.condarc** file using any text editor, I'm using **nano** here

- ***nano .condarc***

copy paste the following lines

```
channels:
- defaults

# Show channel URLs when displaying what is going to be downloaded and
# in 'conda list'. The default is False.
show_channel_urls: True
allow_other_channels: True

proxy_servers:
    http: 10.8.0.1:8080
    https: 10.8.0.1:8080


ssl_verify: False
```

Now let say we have to create a environment myenv with python=3.8

```
conda create -n myenv python=3.8
```

If all the steps done correctly, then the above should work fine.

Script for using conda on the IIT Mandi HPC cluster. Access the latest version of Python without needing to build a Singularity container.

```
#!/bin/bash
#PBS -q gpuq
#PBS -o out.o
#PBS -e out.e
#PBS -N conda
#PBS -l nodes=1:ppn=1
#PBS -l walltime=00:02:00
#PBS -l nodes=n81.cluster.iitmandi.ac.in
#PBS -V

cd ${PBS_O_WORKDIR} # to make sure that we are in the right dir on compute node
echo "Running on: " # on standard output
cat ${PBS_NODEFILE} # env variable for file name containing node details
cat $PBS_NODEFILE > machines.list # also on machines.list file
echo "Program Output begins: "
source ~/miniconda3/bin/activate <environment-name> # to enable myvenv on compute node.
python python_script.py
```