How to create conda environments on Kaya using the latest version of Anaconda3-2024.06.

```
(base) wtraining3@kaya1[~]$ conda create -n s1 python=3.11
Channels:
 - defaults
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /home/wtraining/wtraining3/.conda/envs/s1

  added / updated specs:
    - python=3.11


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    pip-24.0                   |  py311h06a4308_0        3.3 MB
    python-3.11.9              |       h955ad1f_0       32.9 MB
    setuptools-69.5.1          |  py311h06a4308_0        1.3 MB
    wheel-0.43.0               |  py311h06a4308_0        146 KB
    ------------------------------------------------------------
                                   Total:       37.7 MB

The following NEW packages will be INSTALLED:

  _libgcc_mutex     pkgs/main/linux-64::_libgcc_mutex-0.1-main
  _openmp_mutex     pkgs/main/linux-64::_openmp_mutex-5.1-1_gnu
  bzip2             pkgs/main/linux-64::bzip2-1.0.8-h5eee18b_6
  ca-certificates   pkgs/main/linux-64::ca-certificates-2024.3.11-h06a4308_0
  ld_impl_linux-64  pkgs/main/linux-64::ld_impl_linux-64-2.38-h1181459_1
  libffi            pkgs/main/linux-64::libffi-3.4.4-h6a678d5_1
  libgcc-ng         pkgs/main/linux-64::libgcc-ng-11.2.0-h1234567_1
  libgomp           pkgs/main/linux-64::libgomp-11.2.0-h1234567_1
  libstdcxx-ng      pkgs/main/linux-64::libstdcxx-ng-11.2.0-h1234567_1
  libuuid           pkgs/main/linux-64::libuuid-1.41.5-h5eee18b_0
  ncurses           pkgs/main/linux-64::ncurses-6.4-h6a678d5_0
  openssl           pkgs/main/linux-64::openssl-3.0.14-h5eee18b_0
```

```
  pip               pkgs/main/linux-64::pip-24.0-py311h06a4308_0
  python            pkgs/main/linux-64::python-3.11.9-h955ad1f_0
  readline          pkgs/main/linux-64::readline-8.2-h5eee18b_0
  setuptools        pkgs/main/linux-64::setuptools-69.5.1-py311h06a4308_0
  sqlite            pkgs/main/linux-64::sqlite-3.45.3-h5eee18b_0
  tk                pkgs/main/linux-64::tk-8.6.14-h39e8969_0
  tzdata            pkgs/main/noarch::tzdata-2024a-h04d1e81_0
  wheel             pkgs/main/linux-64::wheel-0.43.0-py311h06a4308_0
  xz                pkgs/main/linux-64::xz-5.4.6-h5eee18b_1
  zlib              pkgs/main/linux-64::zlib-1.2.13-h5eee18b_1


Proceed ([y]/n)? y


Downloading and Extracting Packages:

Preparing transaction: done
Verifying transaction: done
Executing transaction: done
#
# To activate this environment, use
#
#     $ conda activate s1
#
# To deactivate an active environment, use
#
#     $ conda deactivate

(base) wtraining3@kaya1[~]$ conda activate s1
(s1) wtraining3@kaya1[~]$ which python3
~/.conda/envs/s1/bin/python3
(s1) wtraining3@kaya1[~]$ python3 -V
Python 3.11.9
```

This creates a new python environment with Python-3.11.

However, when you try with
> conda create –p /group/wtraining/wtraining3/s2'

```
(s1) wtraining3@kaya1[~]$ conda deactivate
(base) wtraining3@kaya1[~]$ conda create -p /group/wtraining/wtraining3/s2 python=3.11
Channels:
```

- defaults
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: done

Package Plan

environment location: /group/wtraining/wtraining3/s2

added / updated specs:
- python=3.11

The following NEW packages will be INSTALLED:

```
_libgcc_mutex      pkgs/main/linux-64::_libgcc_mutex-0.1-main
_openmp_mutex      pkgs/main/linux-64::_openmp_mutex-5.1-1_gnu
bzip2              pkgs/main/linux-64::bzip2-1.0.8-h5eee18b_6
ca-certificates    pkgs/main/linux-64::ca-certificates-2024.3.11-h06a4308_0
ld_impl_linux-64   pkgs/main/linux-64::ld_impl_linux-64-2.38-h1181459_1
libffi             pkgs/main/linux-64::libffi-3.4.4-h6a678d5_1
libgcc-ng          pkgs/main/linux-64::libgcc-ng-11.2.0-h1234567_1
libgomp            pkgs/main/linux-64::libgomp-11.2.0-h1234567_1
libstdcxx-ng       pkgs/main/linux-64::libstdcxx-ng-11.2.0-h1234567_1
libuuid            pkgs/main/linux-64::libuuid-1.41.5-h5eee18b_0
ncurses            pkgs/main/linux-64::ncurses-6.4-h6a678d5_0
openssl            pkgs/main/linux-64::openssl-3.0.14-h5eee18b_0
pip                pkgs/main/linux-64::pip-24.0-py311h06a4308_0
python             pkgs/main/linux-64::python-3.11.9-h955ad1f_0
readline           pkgs/main/linux-64::readline-8.2-h5eee18b_0
setuptools         pkgs/main/linux-64::setuptools-69.5.1-py311h06a4308_0
sqlite             pkgs/main/linux-64::sqlite-3.45.3-h5eee18b_0
tk                 pkgs/main/linux-64::tk-8.6.14-h39e8969_0
tzdata             pkgs/main/noarch::tzdata-2024a-h04d1e81_0
wheel              pkgs/main/linux-64::wheel-0.43.0-py311h06a4308_0
xz                 pkgs/main/linux-64::xz-5.4.6-h5eee18b_1
zlib               pkgs/main/linux-64::zlib-1.2.13-h5eee18b_1
```

Proceed ([y]/n)? y

Downloading and Extracting Packages:

```
Preparing transaction: done
Verifying transaction: done
Executing transaction: done
#
# To activate this environment, use
#
#     $ conda activate /group/wtraining/wtraining3/s2
#
# To deactivate an active environment, use
#
#     $ conda deactivate
```

```
(base) wtraining3@kaya1[~]$ conda activate /group/wtraining/wtraining3/s2
(/group/wtraining/wtraining3/s2) wtraining3@kaya1[~]$ which python3
/usr/bin/python3
(/group/wtraining/wtraining3/s2) wtraining3@kaya1[~]$ python3 -V
Python 3.6.8
```

So that is not Python-3.11 and the path points to the very old default system version of python.

If we check the permissions for the /group/wtraining/wtraining3/s2 environment we created it shows

```
(/group/wtraining/wtraining3/s2) wtraining3@kaya1[~]$ cd /group/wtraining/wtraining3/s2
(/group/wtraining/wtraining3/s2) wtraining3@kaya1[s2]$ ls -al
total 0
drwxrwxr-x 13 wtraining3 wtraining3 0 Jul  9 15:17 .
drwx------ 12 wtraining3 wtraining3 0 Jul  9 15:16 ..
drwxrwxr-x  2 wtraining3 wtraining3 0 Jul  9 15:17 bin
drwxrwxr-x  2 wtraining3 wtraining3 0 Jul  9 15:17 compiler_compat
drwxrwxr-x  2 wtraining3 wtraining3 0 Jul  9 15:17 conda-meta
drwxrwxr-x  2 wtraining3 wtraining3 0 Jul  9 15:17 etc
drwxrwxr-x  9 wtraining3 wtraining3 0 Jul  9 15:17 include
drwxrwxr-x 16 wtraining3 wtraining3 0 Jul  9 15:17 lib
drwxrwxr-x  3 wtraining3 wtraining3 0 Jul  9 15:17 man
drwxrwxr-x 10 wtraining3 wtraining3 0 Jul  9 15:17 share
drwxrwxr-x  3 wtraining3 wtraining3 0 Jul  9 15:17 ssl
drwxrwxr-x  3 wtraining3 wtraining3 0 Jul  9 15:17 x86_64-conda_cos7-linux-gnu
drwxrwxr-x  3 wtraining3 wtraining3 0 Jul  9 15:17 x86_64-conda-linux-gnu
```

But when you look in the bin directory

```
(/group/wtraining/wtraining3/s2) wtraining3@kaya1[s2]$ ls -al bin/py*
lrwxrwxrwx 1 wtraining3 wtraining3      9 Jul  9 15:17 bin/pydoc -> pydoc3.11
lrwxrwxrwx 1 wtraining3 wtraining3      9 Jul  9 15:17 bin/pydoc3 -> pydoc3.11
-rw-rw-r-- 1 wtraining3 wtraining3    105 Jul  9 15:17 bin/pydoc3.11
lrwxrwxrwx 1 wtraining3 wtraining3     10 Jul  9 15:17 bin/python -> python3.11
lrwxrwxrwx 1 wtraining3 wtraining3     10 Jul  9 15:17 bin/python3 -> python3.11
lrwxrwxrwx 1 wtraining3 wtraining3     10 Jul  9 15:17 bin/python3.1 -> python3.11
-rw-rw-r-- 1 wtraining3 wtraining3 24634528 Jul  9 15:17 bin/python3.11
-rw-rw-r-- 1 wtraining3 wtraining3   3448 Jul  9 15:17 bin/python3.11-config
lrwxrwxrwx 1 wtraining3 wtraining3     17 Jul  9 15:17 bin/python3-config -> python3.11-config
```

None of the python commands shown above have executable permissions. I have no idea why, but it is something to do with the “conda create –p” command.

Compared to a conda environment created with “conda create –n" where all the python3 commands are executable see the listing below.

```
(/group/wtraining/wtraining3/s2)$ ls -al ~/.conda/envs/s1/bin/py*
lrwxrwxrwx 1 wtraining3 wtraining3      9 Jul  9 15:12 /home/wtraining/wtraining3/.conda/envs/s1/bin/pydoc ->
pydoc3.11
lrwxrwxrwx 1 wtraining3 wtraining3      9 Jul  9 15:12 /home/wtraining/wtraining3/.conda/envs/s1/bin/pydoc3 ->
pydoc3.11
-rwxrwxr-x 1 wtraining3 wtraining3    116 Jul  9 15:12 /home/wtraining/wtraining3/.conda/envs/s1/bin/pydoc3.11
lrwxrwxrwx 1 wtraining3 wtraining3     10 Jul  9 15:12 /home/wtraining/wtraining3/.conda/envs/s1/bin/python ->
python3.11
lrwxrwxrwx 1 wtraining3 wtraining3     10 Jul  9 15:12 /home/wtraining/wtraining3/.conda/envs/s1/bin/python3 ->
python3.11
lrwxrwxrwx 1 wtraining3 wtraining3     10 Jul  9 15:12 /home/wtraining/wtraining3/.conda/envs/s1/bin/python3.1 ->
python3.11
-rwxrwxr-x 1 wtraining3 wtraining3 24634528 Jul  9 15:12
/home/wtraining/wtraining3/.conda/envs/s1/bin/python3.11
-rwxrwxr-x 1 wtraining3 wtraining3   3481 Jul  9 15:12 /home/wtraining/wtraining3/.conda/envs/s1/bin/python3.11-
config
lrwxrwxrwx 1 wtraining3 wtraining3     17 Jul  9 15:12 /home/wtraining/wtraining3/.conda/envs/s1/bin/python3-
config -> python3.11-config
```

The permissions are correct!

You will need to change the permissions, but this will make the commands available in your $PATH.

```
(/group/wtraining/wtraining3/s2) wtraining3@kaya1[~]$ chmod -R 775 /group/wtraining/wtraining3/s2/bin
```

```
(/group/wtraining/wtraining3/s2) wtraining3@kaya1[~]$ ls -al /group/wtraining/wtraining3/s2/bin/py*
lrwxrwxrwx 1 wtraining3 wtraining3      9 Jul  9 15:17 /group/wtraining/wtraining3/s2/bin/pydoc -> pydoc3.11
lrwxrwxrwx 1 wtraining3 wtraining3      9 Jul  9 15:17 /group/wtraining/wtraining3/s2/bin/pydoc3 -> pydoc3.11
-rwxrwxr-x 1 wtraining3 wtraining3    105 Jul  9 15:17 /group/wtraining/wtraining3/s2/bin/pydoc3.11
lrwxrwxrwx 1 wtraining3 wtraining3     10 Jul  9 15:17 /group/wtraining/wtraining3/s2/bin/python -> python3.11
lrwxrwxrwx 1 wtraining3 wtraining3     10 Jul  9 15:17 /group/wtraining/wtraining3/s2/bin/python3 -> python3.11
lrwxrwxrwx 1 wtraining3 wtraining3     10 Jul  9 15:17 /group/wtraining/wtraining3/s2/bin/python3.1 -> python3.11
-rwxrwxr-x 1 wtraining3 wtraining3 24634528 Jul  9 15:17 /group/wtraining/wtraining3/s2/bin/python3.11
-rwxrwxr-x 1 wtraining3 wtraining3   3448 Jul  9 15:17 /group/wtraining/wtraining3/s2/bin/python3.11-config
lrwxrwxrwx 1 wtraining3 wtraining3     17 Jul  9 15:17 /group/wtraining/wtraining3/s2/bin/python3-config ->
python3.11-config
```

It is a good idea to then deactivate the current environment and logout so you can get to a clean environment.

>conda deactivate

> exit (close the remote session in VS Code)

Login and then activate the conda environment

ssh wtraining3@kaya.hpc.uwa.edu.au
(wtraining3@kaya.hpc.uwa.edu.au) Password:

```
 m   m
 # m"  mmm   m   m   mmm
 #m#   "   #  "m m"  "   #
 # #m  m"""#   #m#   m"""#
 #  "m "mm"#   "#    "mm"#
          m"
          ""
```

Last login: Tue Jul 9 15:34:56 2024 from 10.5.192.7

Activate your conda environment.

```
(base) wtraining3@kaya1[~]$ conda activate /group/wtraining/wtraining3/s2
```

Verify that you have the correct version of Python in your conda environment.

```
(/group/wtraining/wtraining3/s2)$ which python
/group/wtraining/wtraining3/s2/bin/python
(/group/wtraining/wtraining3/s2)$ python -V
Python 3.11.9
(/group/wtraining/wtraining3/s2)$ python3 -V
Python 3.11.9
```

With the correct version of python in the custom conda environment path.

Then next step before you install TensorFlow or PyTorch is to load the cuda module

$ module load cuda/11.8 (or 12.0 once it is installed)

There are 831 different PyTorch packages in conda-forge shown if you search

$ conda search –c conda-forge pytorch

Assuming you are only interested in the latest release 2.3.1

(s1)$ conda search -c conda-forge pytorch=2.3.1
Loading channels: done

Name Version Build Channel
pytorch 2.3.1 cpu_generic_py310ha4c588e_0 conda-forge pytorch 2.3.1 cpu_generic_py311h8ca351a_0 conda-forge pytorch 2.3.1 cpu_generic_py312h2f1fc2b_0 conda-forge pytorch 2.3.1 cpu_generic_py38h1fa1760_0 conda-forge pytorch 2.3.1 cpu_generic_py39he75b87c_0 conda-forge pytorch 2.3.1 cpu_mkl_py310h75865b9_100 conda-forge

pytorch 2.3.1 cpu_mkl_py311hcb16b95_100 conda-forge
pytorch 2.3.1 cpu_mkl_py312h3b258cc_100 conda-forge
pytorch 2.3.1 cpu_mkl_py38h51400c9_100 conda-forge
pytorch 2.3.1 cpu_mkl_py39h85c4de8_100 conda-forge
pytorch 2.3.1 cuda118_py310he8d5cbe_300 conda-forge
pytorch 2.3.1 cuda118_py311h0047a46_300 conda-forge
pytorch 2.3.1 cuda118_py312h409cda2_300 conda-forge
pytorch 2.3.1 cuda118_py38h63640cd_300 conda-forge
pytorch 2.3.1 cuda118_py39hd3e083d_300 conda-forge
pytorch 2.3.1 cuda120_py310h2c91c31_300 conda-forge
pytorch 2.3.1 cuda120_py311hf6aebf0_300 conda-forge
pytorch 2.3.1 cuda120_py312h26b3cf7_300 conda-forge
pytorch 2.3.1 cuda120_py38hc4689d7_300 conda-forge
pytorch 2.3.1 cuda120_py39h17b67e0_300 conda-forge

The highlighted versions are the CUDA build versions

- cuda118 refers to cuda-11.8
- cuda120 refers to cuda-12.0

Each cuda version is for specific versions of python as well. You will need to know what version of cuda is required and the python version. Then explicitly install the correct build version!

If you just do a basic conda install you will not get the correct build.

```
(s1) $ conda install pytorch
Channels:
 - defaults
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment done

## Package Plan ##

  environment location: /home/wtraining/wtraining3/.conda/envs/s1

  added / updated specs:
    - pytorch

The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    filelock-3.13.1            |  py311h06a4308_0          24 KB
    fsspec-2024.3.1            |  py311h06a4308_0         379 KB
    gmp-6.2.1                  |       h295c915_3         544 KB
    gmpy2-2.1.2                |  py311hc9b5ff0_0         191 KB
    jinja2-3.1.4               |  py311h06a4308_0         360 KB
    markupsafe-2.1.3           |  py311h5eee18b_0          25 KB
    mkl-service-2.4.0          |  py311h5eee18b_1          54 KB
    mkl_fft-1.3.8              |  py311h5eee18b_0         225 KB
    mkl_random-1.2.4           |  py311hdb19cb5_0         316 KB
    mpc-1.1.0                  |       h10f8cd9_1          90 KB
    mpfr-4.0.2                 |       hb69a4c5_1         487 KB
    mpmath-1.3.0               |  py311h06a4308_0         1.0 MB
    networkx-3.3               |  py311h06a4308_0         3.1 MB
    numpy-1.26.4               |  py311h08b1b3b_0          10 KB
    numpy-base-1.26.4          |  py311hf175353_0         8.3 MB
    pytorch-2.3.0              |cpu_py311ha0631a7_0        76.8 MB
    sympy-1.12                 |  py311h06a4308_0        14.4 MB
    typing_extensions-4.11.0   |  py311h06a4308_0          73 KB
    ------------------------------------------------------------
                                           Total:       106.2 MB
```

So that is a non-gpu build and not the latest release, but it did pick up the right python version.

Even with the cuda module loaded it is not enough. You need the conda channel or you may not get the right version

```
(s1)$ module load cuda/11.8
(s1)$ conda install pytorch=2.3.1
Channels:
 - defaults
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: failed

PackagesNotFoundError: The following packages are not available from current channels:

  - pytorch=2.3.1*

Current channels:

  - defaults

To search for alternate channels that may provide the conda package you are
looking for, navigate to

    https://anaconda.org

and use the search bar at the top of the page.
```

Still with *conda forge* and the cuda module loaded

```
(s1)$ conda install -c conda-forge pytorch=2.3.1
Channels:
 - conda-forge
 - defaults
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /home/wtraining/wtraining3/.conda/envs/s1

  added / updated specs:
    - pytorch=2.3.1
```

The following packages will be downloaded:

package	build		
_libgcc_mutex-0.1	conda_forge	3 KB	conda-forge
_openmp_mutex-4.5	2_kmp_llvm	6 KB	conda-forge
ca-certificates-2024.7.4	hbcca054_0	151 KB	conda-forge
filelock-3.15.4	pyhd8ed1ab_0	17 KB	conda-forge
fsspec-2024.6.1	pyhff2d567_0	130 KB	conda-forge
icu-73.2	h59595ed_0	11.5 MB	conda-forge
jinja2-3.1.4	pyhd8ed1ab_0	109 KB	conda-forge
libabseil-20240116.2	cxx17_h59595ed_0	1.2 MB	conda-forge
libblas-3.9.0	22_linux64_openblas	14 KB	conda-forge
libcblas-3.9.0	22_linux64_openblas	14 KB	conda-forge
libgcc-ng-14.1.0	h77fa898_0	822 KB	conda-forge
libgfortran-ng-14.1.0	h69a702a_0	49 KB	conda-forge
libgfortran5-14.1.0	hc5f4f2c_0	1.4 MB	conda-forge
libgomp-14.1.0	h77fa898_0	446 KB	conda-forge
libhwloc-2.11.0	default_h5622ce7_1000	2.3 MB	conda-forge
libiconv-1.17	hd590300_2	689 KB	conda-forge
liblapack-3.9.0	22_linux64_openblas	14 KB	conda-forge
libopenblas-0.3.27	pthreads_hac2b453_1	5.3 MB	conda-forge
libprotobuf-4.25.3	h08a7969_0	2.7 MB	conda-forge
libstdcxx-ng-14.1.0	hc0a3c3a_0	3.7 MB	conda-forge
libtorch-2.3.1	cpu_mkl_h0bb0d08_100	47.5 MB	conda-forge
libuv-1.48.0	hd590300_0	879 KB	conda-forge
libxml2-2.12.7	hc051c1a_1	688 KB	conda-forge
libzlib-1.2.13	h4ab18f5_6	60 KB	conda-forge
llvm-openmp-18.1.7	ha31de31_0	55.9 MB	conda-forge
markupsafe-2.1.5	py311h459d7ec_0	27 KB	conda-forge
mkl-2023.2.0	h84fe81f_50496	156.8 MB	conda-forge
mpmath-1.3.0	pyhd8ed1ab_0	428 KB	conda-forge
networkx-3.3	pyhd8ed1ab_1	1.1 MB	conda-forge
numpy-2.0.0	py311h1461c94_0	8.5 MB	conda-forge
openssl-3.3.1	h4ab18f5_1	2.8 MB	conda-forge
python_abi-3.11	2_cp311	5 KB	conda-forge
pytorch-2.3.1	cpu_mkl_py311hcb16b95_100	31.9 MB	conda-forge
sleef-3.5.1	h9b69904_2	1.5 MB	conda-forge
sympy-1.12.1	pyh04b8f61_3	4.0 MB	conda-forge
tbb-2021.12.0	h434a139_2	188 KB	conda-forge
typing_extensions-4.12.2	pyha770c72_0	39 KB	conda-forge
zlib-1.2.13	h4ab18f5_6	91 KB	conda-forge
zstd-1.5.6	ha6fb4c9_0	542 KB	conda-forge

Total: 343.6 MB

So even with the cuda module loaded and conda using the right version of python, you still do not get a gpu build version of pytorch.

The correct way to install the package is with the build version!

```
$ conda install "conda-forge/linux-64::pytorch 2.3.1 cuda118_py311h0047a46_300"
Channels:
 - defaults
 - conda-forge
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /group/wtraining/wtraining3/s2
  added / updated specs:
    - conda-forge/linux-64::pytorch==2.3.1=cuda118_py311h0047a46_300


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    _openmp_mutex-4.5          |      2_kmp_llvm          6 KB  conda-forge
    cudnn-8.9.7.29             |      hbc23b4c_3       443.9 MB  conda-forge
    filelock-3.13.1            |  py311h06a4308_0         24 KB
    fsspec-2024.3.1            |  py311h06a4308_0        379 KB
    gmp-6.2.1                  |      h295c915_3        544 KB
    gmpy2-2.1.2                |  py311hc9b5ff0_0        191 KB
    jinja2-3.1.4               |  py311h06a4308_0        360 KB
    libabseil-20240116.2       | cxx17_h6a678d5_0        1.3 MB
    libblas-3.9.0              |22_linux64_openblas         14 KB  conda-forge
    libcblas-3.9.0             |22_linux64_openblas         14 KB  conda-forge
    libgfortran-ng-14.1.0      |      h69a702a_0         49 KB  conda-forge
    libgfortran5-14.1.0        |      hc5f4f2c_0        1.4 MB  conda-forge
    liblapack-3.9.0            |22_linux64_openblas         14 KB  conda-forge
    libmagma-2.7.2             |      h09b5827_2       265.8 MB  conda-forge
    libmagma_sparse-2.7.2      |      h09b5827_3         7.1 MB  conda-forge
    libopenblas-0.3.27         |pthreads_hac2b453_1         5.3 MB  conda-forge
    libprotobuf-4.25.3         |      he621ea3_0         2.8 MB
    libtorch-2.3.1             |cuda118_h7aef8b2_300       455.3 MB  conda-forge
    libuv-1.48.0               |      hd590300_0         879 KB  conda-forge
    llvm-openmp-18.1.7         |      ha31de31_0        55.9 MB  conda-forge
    mkl-2023.2.0               |   h84fe81f_50496       156.8 MB  conda-forge
    mpc-1.1.0                  |      h10f8cd9_1         90 KB
```

```
mpfr-4.0.2              |      hb69a4c5_1        487 KB
mpmath-1.3.0            |  py311h06a4308_0       1.0 MB
networkx-3.3            |  py311h06a4308_0       3.1 MB
pytorch-2.3.1           |cuda118_py311h0047a46_300      32.2 MB  conda-forge
sleef-3.5.1             |      h9b69904_2        1.5 MB  conda-forge
sympy-1.12              |  py311h06a4308_0       14.4 MB
zstd-1.5.6              |      ha6fb4c9_0        542 KB  conda-forge
------------------------------------------------------------
                                       Total:        1.42 GB
```

The following steps listed below should help you set up the right environment to run pytorch or TensorFlow on a GPU (graphics processing units).

Summary of commands

#Create new Conda environment in $MYGROUP on Kaya

$(base)$ conda create -p /group/wtraining/wtraining3/s2 python=3.11

#Change the permissions
$(base)$ chmod -R 775 /group/wtraining/wtraining3/s2/bin
Recommend that you logout and log back-in to fix any environment issue

Activate the Environment

$(base)~] $ conda activate /group/wtraining/wtraining3/s2

#Verify you are getting the correct python version

$(/group/wtraining/wtraining3/s2/)$ which python
/group/wtraining/wtraining3/s2/bin/python
$(/group/wtraining/wtraining3/s2)$ python -V
Python 3.11.9
$(/group/wtraining/wtraining3/s2)$ python3 -V
Python 3.11.9

##

Need to perform the following steps directly on a Compute Node and not on the Login Node. There is an environment issue on the login node that I have not work out. It just works on the Compute nodes without any issues.

To get an interactive session on a compute node with a GPU you can use this command

salloc -N 1 --time=01:00:00 --partition=gpu --mem=200G --gres=gpu:v100:1

Activate the Environment on the compute node

$(base)~] $ conda activate /group/wtraining/wtraining3/s2

#Search for the latest build version of PyTorch (or TensorFlow)

$(s2)$ conda search -c conda-forge pytorch
or
$(s2)$ conda search -c conda-forge tensorflow

conda install "conda-forge/linux-64::tensorflow 2.14.0 cuda118py311heb1bdc4_0"

#Load the Cuda module
(s2)$ module load cuda/11.8

#Install pytorch or tensor and specify the correct build version for both the cuda libraries and python version!

(s2)$ conda install "conda-forge/linux-64::pytorch 2.3.1 cuda118_py311h0047a46_300"

#Note The TensorFlow environment is done the exact same way

NOTE ### there are ***NO equal signs used in the command***

(s2$)conda install "conda-forge/linux-64::tensorflow 2.14.0 cuda118py311heb1bdc4_0"