```
(base) pdiaz$  ssh pdiaz@ed6.hpc.nrel.gov
*****************************************************
                          NOTICE TO USERS

This is a Federal computer or information system and is the property of the
United States Government.  It is for authorized use only.  By using this
information system, or connecting any device to this information system, the
user acknowledges, understands and consents to certain identified actions and agrees:

  * that user has no reasonable expectation of privacy regarding communications
    or data transmitted or stored on this information system or any devices
    connected to this information system.

  * that any or all uses of this information system and all files transmitted,
    stored or connected to this information system may be intercepted, monitored,
    recorded, copied and searched and may be used or disclosed to law enforcement
    or other Government agencies, as deemed appropriate by the Department of Energy
    or as mandated by law.

  * to be bound by the requirements for use of Government information systems
    consistent with DOE Order 203.1 and any other applicable DOE Order or directive
    regarding use of DOE information systems.

  * that any unauthorized or improper use of Government information systems may
    result in limitations placed on the use of Government information systems,
    disciplinary or adverse actions, criminal penalties, and/or
    financial liability for the cost of such improper use.

To the extent that the user has any questions concerning the use of Government
information systems, the user should consult with their supervisor or other
appropriate management personnel.  LOG OFF IMMEDIATELY if you do not agree
to the conditions stated in this warning.
****************************************************
pdiaz@ed6.hpc.nrel.gov's password:
Last login: Fri Apr 23 12:45:52 2021 from ssl-vpn-10-10-141-40.nrel.gov


The NREL High Performance Computing Center systems
may only contain data related to scientific research.

This system may only contain data that is categorized as:
  low
  non-sensitive

This system may not store or process data that is:
  proprietary
  export controlled

By logging into this system, you agree to the HPC Center terms and policies:
  http://hpc.nrel.gov/users/policies

 *** Notice: Mail List for Support requests ***

Send email to hpc-help@nrel.gov for HPC support requests and trouble reports.

Contact the NREL Service Center For workstation and laptop service requests:
  service.center@nrel.gov  303-275-4171

[pdiaz@ed6 ~]$ cd ~/
[pdiaz@ed6 ~]$ git clone https://github.com/NREL/HPC
Cloning into 'HPC'...
remote: Enumerating objects: 2043, done.
remote: Counting objects: 100% (299/299), done.
remote: Compressing objects: 100% (229/229), done.
remote: Total 2043 (delta 130), reused 161 (delta 58), pack-reused 1744
Receiving objects: 100% (2043/2043), 101.00 MiB | 53.41 MiB/s, done.
Resolving deltas: 100% (890/890), done.
[pdiaz@ed6 ~]$ cd ./HPC/workshops/Optimized_TF/
[pdiaz@ed6 Optimized_TF]$ module purge
[pdiaz@ed6 Optimized_TF]$ module use /nopt/nrel/apps/modules/test/modulefiles/
[pdiaz@ed6 Optimized_TF]$ module load conda
[pdiaz@ed6 Optimized_TF]$ module load gcc/7.4.0
[pdiaz@ed6 Optimized_TF]$ module load cudnn/8.0.5/cuda-10.2
[pdiaz@ed6 Optimized_TF]$
[pdiaz@ed6 Optimized_TF]$
[pdiaz@ed6 Optimized_TF]$
[pdiaz@ed6 Optimized_TF]$ module avail

------------------------------------------------------------------------- /nopt/nrel/apps/modules/test/modulefiles --------------------------------------------------------------------------
   ansys/em2020R2           converge/3.0.16       (D)    cudnn/8.1.1/cuda-11.2             helics/helics-2.4.1_light          idl/8.7                    nwchem/7.0.0                               (D)    openmpi/4.0.x-65219eb/gcc-7.3.0                  singularity-container/3.5.3
   ansys/2019R3             cuda/9.0.176                 cudnn/cudnn_opencv                helics/helics-2.5_debug            intel-mpi/2019.0.1         openmpi/1.10.7/gcc-8.4.0                   (D)    openmpi/4.1.0-gcc-8.4.0/gcc-8.4.0-j15            singularity-container/3.6.4 (D)
   ansys/2020R2             cuda/10.0.130b               dakota/6.9.0                      helics/helics-2.5_openmpi_nb       lammps/20200303     (D)    openmpi/2.1.6/gcc-7.3.0                           openmpi/4.1.0-gcc-8.4.0/gcc-8.4.0     (D)        spack/0.12.1
   ansys/2021R1      (D)    cuda/10.0.130                darshan-runtime/3.2.1             helics/helics-2.5_openmpi          mathematica/12.1           openmpi/3.1.3-nopmi/gcc-7.3.0                     pgi64/16.5                                       starccm/15.06.008
   cmake/3.16.5             cuda/10.1.168                darshan-util/3.2.1                helics/helics-2.6_openmpi_d        matlab/R2019a              openmpi/3.1.3-noslurm/gcc-7.3.0                   pgi64/18.10_llvm                                 vasp/5.4.4_raptor
   cmake/3.18.2      (D)    cuda/10.2.89          (L)    gaussian/G16A                     helics/helics-2.6_openmpi          matlab/R2019b              openmpi/3.1.3-noslurm_nomxm/gcc-7.3.0             pgi64/18.10                                      vasp/6.1.0
   comp-intel/2019.0.1      cuda/11.2             (D)    gaussian/G16C_GPU                 helics/helics-2.6.1_dev            matlab/R2020a              openmpi/3.1.3-noslurmk/gcc-7.3.0                  pgi64/19.7                                       xpressmp/8.8.0              (D)
   comp-intel/2020.1        cudnn/7.4.2/cuda-9.0         gaussian/G16C              (D)    helics/helics-2.6.1_intel          matlab/R2020b       (D)    openmpi/3.1.3-noslurmk/intel-18.0.3        (D)    pgi64/20.1                            (D)
   comsol/5.6        (D)    cudnn/7.4.2/cuda-9.2         git-lfs/2.11.0                    helics/helics-2.6.1_openmpi        mpt/2.23            (D)    openmpi/3.1.3-slurm19/gcc-7.3.0                   q-chem/5.3_MPI
   conda/4.8.3              cudnn/7.4.2/cuda-10.0 (D)    helics/helics-2.3.1_openmpi       helics/plexos-helics-mod           nco/4.7.9                  openmpi/4.0.4/gcc+cuda                            quantum-espresso/6.4.1
   conda/2019.10            cudnn/8.0.5/cuda-10.2 (L)    helics/helics-2.4_openmpi         helics/plexos-helics        (D)    nwchem/7.0.0-intel20       openmpi/4.0.x-65219eb-ucx/gcc-7.3.0               singularity-container/3.2.1

------------------------------------------------------------------------ /nopt/nrel/apps/modules/default/modulefiles -------------------------------------------------------------------------
   abaqus/abaqus2018            comsol/5.5                       gaussian/G16C                        hdf5/1.10.7/gcc-ompi                mesa/13.0.3                        openmpi/1.10.7/gcc-8.4.0        plexos/8.000R03                    wrf/4.1.3/intel-20.1.217-mpi
   ansys/2019R3                 conda/mini_py37_4.8.3    (L,D)   gcc/5.5.0                            hdf5/1.10.7/gcc-serial              mkl/2020.1.217                     openmpi/3.1.6/gcc-8.4.0         plexos/8.0                         wrf/4.2.1/intel-20.1.217-mpi
   arm/20.1                     converge/2.4.23                  gcc/6.5.0                            hdf5/1.10.7/intel-impi              mono/4.0.4.1                       openmpi/4.0.4/gcc-8.4.0  (D)    plexos/8.100R02                    xpressmp/7.8.0
   arm/20.2              (D)    cuda/10.2.89                     gcc/7.4.0                  (L)       hdf5/1.10.7/intel-serial    (D)     mono/4.6.2.7              (D)      paraview/osmesa-5.6             plexos/8.200R01                    xpressmp/8.0.4
   avizo/2019.3                 cudnn/7.4.2/cuda-10.0            gcc/8.4.0                            hdf5/1.12.0/intel-impi              mono/5.4.0.167                     paraview/osmesa-5.8             pnetcdf/1.12.1/gcc-ompi            xpressmp/8.2
   avizo/2020.2          (D)    cudnn/7.6.1/cuda-10.1            gcc/9.3.0                            hdf5/1.12.0/intel-serial    (D)     mono/6.8.0.105                     paraview/osmesa-5.9             pnetcdf/1.12.1/intel-impi   (D)    xpressmp/8.5.6
   boost/1.73.0/gcc             dav_cuda/10.1.168                gcc/10.1.0                 (D)       helics/helics-2.6.1_intel           mpt/2.22                           paraview/5.6.0           (D)    q-chem/5.3                  (D)    xpressmp/8.8.0
   boost/1.73.0/intel    (D)    dineof/3.0/intel                 gsl/2.5/gcc                          helics/helics-2.6.1_openmpi         ncl/6.6.2                          pgi64/18.10_llvm                singularity-container/3.6.1
   centos/7.7                   fftw/3.3.8/gcc-serial            gurobi/9.0.2                         idl/8.3                     (D)     ncview/2.1.8                       pgi64/18.10                     starccm/13.06.012           (D)
   check/0.12.0                 fftw/3.3.8/intel-impi            hdf5/1.10.6/gcc-ompi                 intel-mpi/2020.1.217        (D)     netcdf-c/4.7.3/gcc-mpi             pgi64/20.1                      starccm/15.06.008
   cmake/3.12.3                 fftw/3.3.8/intel-threaded (D)    hdf5/1.10.6/gcc-serial               lammps/20200303                     netcdf-c/4.7.4/intel               plexos/7.300.4                  vasp/5.4.4_centos77
   cmg/2020.101                 gams/31.1.0                      hdf5/1.10.6/intel-impi               llvm/3.9.1                          netcdf-f/4.5.2/gcc-mpi             plexos/7.400.2           (D)    vasp/6.1.1
   comp-intel/2020.1.217 (D)    gaussian/G16C_GPU                hdf5/1.10.6/intel-serial (D)         matlab/R2020a                       netcdf-f/4.5.3/intel-serial        plexos/7.500.2                  vasp/6.1.2                  (D)

  Where:
   L:  Module is loaded
   D:  Default Module

Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".


[pdiaz@ed6 Optimized_TF]$ conda env create -f py38tf24.yml
Collecting package metadata (repodata.json): done
Solving environment: done
Preparing transaction: done
Verifying transaction: done
Executing transaction: done
Installing pip dependencies: \ Ran pip subprocess with arguments:
['/home/pdiaz/.conda-envs/py38tf24/bin/python', '-m', 'pip', 'install', '-U', '-r', '/home/pdiaz/HPC/workshops/Optimized_TF/condaenv.gt6p97hq.requirements.txt']
Pip subprocess output:
Collecting numpy==1.18.5
  Using cached numpy-1.18.5-cp38-cp38-manylinux1_x86_64.whl (20.6 MB)
Collecting scipy==1.4.1
  Using cached scipy-1.4.1-cp38-cp38-manylinux1_x86_64.whl (26.0 MB)
Collecting ai-benchmark
  Using cached ai_benchmark-0.1.2-py3-none-any.whl (21.5 MB)
Collecting pillow
  Using cached Pillow-8.2.0-cp38-cp38-manylinux1_x86_64.whl (3.0 MB)
Collecting psutil
  Using cached psutil-5.8.0-cp38-cp38-manylinux2010_x86_64.whl (296 kB)
Requirement already satisfied: setuptools in /home/pdiaz/.conda-envs/py38tf24/lib/python3.8/site-packages (from ai-benchmark->-r /home/pdiaz/HPC/workshops/Optimized_TF/condaenv.gt6p97hq.requirements.txt (line 3)) (52.0.0.post20210125)
Requirement already satisfied: requests in /home/pdiaz/.conda-envs/py38tf24/lib/python3.8/site-packages (from ai-benchmark->-r /home/pdiaz/HPC/workshops/Optimized_TF/condaenv.gt6p97hq.requirements.txt (line 3)) (2.25.1)
Collecting py-cpuinfo
  Using cached py_cpuinfo-8.0.0-py3-none-any.whl
Requirement already satisfied: idna<3,>=2.5 in /home/pdiaz/.conda-envs/py38tf24/lib/python3.8/site-packages (from requests->ai-benchmark->-r /home/pdiaz/HPC/workshops/Optimized_TF/condaenv.gt6p97hq.requirements.txt (line 3)) (2.10)
Requirement already satisfied: urllib3<1.27,>=1.21.1 in /home/pdiaz/.conda-envs/py38tf24/lib/python3.8/site-packages (from requests->ai-benchmark->-r /home/pdiaz/HPC/workshops/Optimized_TF/condaenv.gt6p97hq.requirements.txt (line 3)) (1.26.4)
Requirement already satisfied: certifi>=2017.4.17 in /home/pdiaz/.conda-envs/py38tf24/lib/python3.8/site-packages (from requests->ai-benchmark->-r /home/pdiaz/HPC/workshops/Optimized_TF/condaenv.gt6p97hq.requirements.txt (line 3)) (2020.12.5)
Requirement already satisfied: chardet<5,>=3.0.2 in /home/pdiaz/.conda-envs/py38tf24/lib/python3.8/site-packages (from requests->ai-benchmark->-r /home/pdiaz/HPC/workshops/Optimized_TF/condaenv.gt6p97hq.requirements.txt (line 3)) (3.0.4)
Installing collected packages: py-cpuinfo, psutil, pillow, numpy, scipy, ai-benchmark
  Attempting uninstall: numpy
    Found existing installation: numpy 1.20.1
    Uninstalling numpy-1.20.1:
      Successfully uninstalled numpy-1.20.1
  Attempting uninstall: scipy
    Found existing installation: scipy 1.6.2
    Uninstalling scipy-1.6.2:
      Successfully uninstalled scipy-1.6.2
Successfully installed ai-benchmark-0.1.2 numpy-1.18.5 pillow-8.2.0 psutil-5.8.0 py-cpuinfo-8.0.0 scipy-1.4.1

done
#
# To activate this environment, use
#
#     $ conda activate py38tf24
#
# To deactivate an active environment, use
#
#     $ conda deactivate
```

```
(pdiaz@ed6 Optimized_TF)$ conda info --envs
# conda environments:
#
py38tf24                 /home/pdiaz/.conda-envs/py38tf24
speed_env                /home/pdiaz/.conda-envs/speed_env
base                  *  /opt/nrel/apps/anaconda/mini_py37_4.8.3

(pdiaz@ed6 Optimized_TF)$ source activate py38tf24
(/home/pdiaz/.conda-envs/py38tf24) [pdiaz@ed6 Optimized_TF]$ pip install --upgrade --no-deps --force-reinstall /opt/nrel/apps/wheels/tensorflow-2.4.0-cp38-cp38-linux_x86_64.whl
Processing /opt/nrel/apps/wheels/tensorflow-2.4.0-cp38-cp38-linux_x86_64.whl
Installing collected packages: tensorflow
  Attempting uninstall: tensorflow
    Found existing installation: tensorflow 2.4.1
    Uninstalling tensorflow-2.4.1:
      Successfully uninstalled tensorflow-2.4.1
Successfully installed tensorflow-2.4.0
(/home/pdiaz/.conda-envs/py38tf24) [pdiaz@ed6 Optimized_TF]$ python3 -c "import tensorflow as tf; print(tf.reduce_sum(tf.random.normal([1000, 1000])))"
2021-04-23 12:54:27.929043: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcudart.so.10.2
2021-04-23 12:54:32.146061: I tensorflow/compiler/jit/xla_cpu_device.cc:41] Not creating XLA devices, tf_xla_enable_xla_devices not set
2021-04-23 12:54:32.148901: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcuda.so.1
2021-04-23 12:54:32.154852: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1720] Found device 0 with properties:
pciBusID: 0000:37:00.0 name: Quadro GV100 computeCapability: 7.0
coreClock: 1.627GHz coreCount: 80 deviceMemorySize: 31.75GiB deviceMemoryBandwidth: 810.62GiB/s
2021-04-23 12:54:32.154916: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcudart.so.10.2
2021-04-23 12:54:32.203874: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcublas.so.10
2021-04-23 12:54:32.203952: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcublasLt.so.10
2021-04-23 12:54:32.249637: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcufft.so.10
2021-04-23 12:54:32.301669: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcurand.so.10
2021-04-23 12:54:32.348274: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcusolver.so.10
2021-04-23 12:54:32.383309: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcusparse.so.10
2021-04-23 12:54:32.400977: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcudnn.so.8
2021-04-23 12:54:32.402631: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1862] Adding visible gpu devices: 0
2021-04-23 12:54:32.405529: I tensorflow/compiler/jit/xla_gpu_device.cc:99] Not creating XLA devices, tf_xla_enable_xla_devices not set
2021-04-23 12:54:32.406377: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1720] Found device 0 with properties:
pciBusID: 0000:37:00.0 name: Quadro GV100 computeCapability: 7.0
coreClock: 1.627GHz coreCount: 80 deviceMemorySize: 31.75GiB deviceMemoryBandwidth: 810.62GiB/s
2021-04-23 12:54:32.406432: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcudart.so.10.2
2021-04-23 12:54:32.406456: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcublas.so.10
2021-04-23 12:54:32.406482: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcublasLt.so.10
2021-04-23 12:54:32.406503: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcufft.so.10
2021-04-23 12:54:32.406521: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcurand.so.10
2021-04-23 12:54:32.406536: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcusolver.so.10
2021-04-23 12:54:32.406553: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcusparse.so.10
2021-04-23 12:54:32.406568: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcudnn.so.8
2021-04-23 12:54:32.407981: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1862] Adding visible gpu devices: 0
2021-04-23 12:54:32.408020: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcudart.so.10.2
2021-04-23 12:54:33.117530: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1261] Device interconnect StreamExecutor with strength 1 edge matrix:
2021-04-23 12:54:33.117579: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1267]      0
2021-04-23 12:54:33.117594: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1280] 0:   N
2021-04-23 12:54:33.119952: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1406] Created TensorFlow device (/job:localhost/replica:0/task:0/device:GPU:0 with 15633 MB memory) -> physical GPU (device: 0, name: Quadro GV100, pci bus id: 0000:37:00.0, compute capability: 7.0)
tf.Tensor(-377.17816, shape=(), dtype=float32)
(/home/pdiaz/.conda-envs/py38tf24) [pdiaz@ed6 Optimized_TF]$
```