HPC Instruction

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1. Download NYU VPN
   https://www.nyu.edu/life/information-technology/infrastructure/network-services/vpn.html

2. Access HPC
   https://sites.google.com/nyu.edu/nyu-hpc/accessing-hpc?authuser=0
   `ssh <NYU_NetID>@greene.hpc.nyu.edu`

3. Greene Introdution
   https://sites.google.com/nyu.edu/nyu-hpc/home?authuser=0

4. Slurm Tutorial
   https://sites.google.com/nyu.edu/nyu-hpc/training-support/general-hpc-topics/slurm-main-commands
   https://sites.google.com/nyu.edu/nyu-hpc/training-support/tutorials/slurm-tutorial

   Basic Commands:
   # Check job status
   `squeue -u $USER`
   # Cancel a job
   `scancel JOBID`

5. Graphical User Interface (GUI) Tools
   https://ood.hpc.nyu.edu/

6. Availble GPUs
   There are 200 GPU hours for everyone. The job will be canceled if there is low GPU usage for 2 hours.
   partitions = {"n1s8-v100-1", "n1s8-t4-1", "n1s8-p100-1" }

7. Singularity with Miniconda
   https://sites.google.com/nyu.edu/nyu-hpc/hpc-systems/greene/software/singularity-with-miniconda

8. Squash File System for image data
   https://sites.google.com/nyu.edu/nyu-hpc/hpc-systems/hpc-storage/data-management/squash-file-system-and-singularity

Example:

```
ssh burst

# Total GPU hours
sacctmgr list assoc format=user,qos,defaultqos,account%20,GrpTRESMins%30 where account=bmsc_ga_4493 user=$USER

# GPU hours used
sshare --format=user,account,GrpTRESRaw%120 --account=bmsc_ga_4493 --user=$USER

# Run an interactive job
sbatch --account=bmsc_ga_4493 --partition=interactive --time=04:00:00 --wrap "sleep infinity"

squeue -u $USER

# Google Cloud Platform (different directory from Greene)
ssh NODE # use the node in your NODELIST, e.g. ssh b-9-1

# Create a pytorch environment using Singularity and Anaconda
mkdir /scratch/$USER/DL4Med
cd /scratch/$USER/DL4Med

scp -rp greene-dtn:/scratch/work/public/overlay-fs-ext3/overlay-7.5GB-300K.ext3.gz .

gunzip overlay-7.5GB-300K.ext3.gz

singularity exec --overlay overlay-7.5GB-300K.ext3 /share/apps/images/cuda11.3.0-cudnn8-devel-ubuntu20.04.sif /bin/bash

wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh

sh Miniconda3-latest-Linux-x86_64.sh -b -p /ext3/miniconda3

vim  /ext3/env.sh
# Create a wrapper script /ext3/env.sh using vim (basic vim commands), paste the following lines, then [‘esc’] and ‘:wq’
#!/bin/bash
source /ext3/miniconda3/etc/profile.d/conda.sh
export PATH=/ext3/miniconda3/bin:$PATH
export PYTHONPATH=/ext3/miniconda3/bin:$PATH

# Activate conda environment and install packages
```

```
source /ext3/env.sh
conda update -n base conda -y
conda clean --all --yes
conda install pip
conda install ipykernel
pip3 install torch==1.10.2+cu113 torchvision==0.11.3+cu113 \
torchaudio==0.10.2+cu113 -f https://download.pytorch.org/whl/cu113/torch_stable.html
pip3 install jupyter jupyterhub pandas matplotlib scipy scikit-learn scikit-image Pillow


# Exit the Singularity container and then rename the overlay image
exit
mv overlay-7.5GB-300K.ext3 DL4Med_pytorch.ext3

# Copy the Jupyter Notebook script from Greene (upload the file first)
scp -rp greene-dtn:/scratch/$USER/run-jupyter-gpu-HW2.sbatch .

# Run Jupyter Notebook, use the HW2 script for HW2, it incluses the image data
# Use cpu scripts if you don’t need gpu to run the models
sbatch run-jupyter-gpu-HW2.sbatch
squeue -u $USER
cat slurm-xxxxx.out

# Run in a new terminal, then open the link
ssh -L xxxxx:localhost:xxxxx NETID@greene.hpc.nyu.edu

# Somtimes the v100 GPUs are not available, modify the run-jupyter-gpu.sbatch file
#SBATCH --gres=gpu:t4:1
#SBATCH --partition=n1s8-t4-1
Or
#SBATCH --gres=gpu:p100:1
#SBATCH --partition=n1s8-p100-1
```