HPC Instruction

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 Introduction
   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
   # 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. Data Transfer (from your local PC or Google Drive)
   PC: scp -rp images.gz <NetID>@greene-dtn.hpc.nyu.edu:/scratch/<NetID>
   https://sites.google.com/nyu.edu/nyu-hpc/hpc-systems/hpc-storage/data-management/data-transfers/transferring-cloud-storage-data-with-rclone

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

9. 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
```

Working with Data for Projects

1. Data transfer from your local PC
   `scp -rp images.gz <NetID>@greene-dtn.hpc.nyu.edu:/scratch/<NetID>`

2. Data transfer from your Google Drive
   You can also follow the instructions here.
   DON'T run 'ssh burst' after login to Greene
   ```
   module load rclone/1.53.3
   rclone config
   n
   remote1
   13
   <Enter>
   <Enter>
   1
   <Enter>
   <Enter>
   n
   n
   # Go to the link and copy the authorization code
   <authorization code>
   n
   y
   q
   # Copy data from your Google Drive
   rclone copy remote1:<GoogleDriveDataPath> ./Data
   ```

3. Optional: Squash File System and Singularity
   If you have many tiny files as fixed datasets, please make squashFS files to work with Singularity.
   You can also follow the instructions here.
   ```
   # Set access permissions for <images> folder
   find images -type d -exec chmod 755 {} \;
   find images -type f -exec chmod 644 {} \;
   # Convert to a single squashFS file
   mksquashfs images images.sqf  -keep-as-directory
   ```

4. Data transfer from Greene to GCP
   Login to GCP then transfer the data
   `scp -rp greene-dtn:/scratch/$USER/images.sqf .`

5. Sbatch file to run the model

```
#!/bin/bash

#SBATCH --job-name=Model
#SBATCH --nodes=1
#SBATCH --gres=gpu:v100:1
#SBATCH --time=24:00:00
#SBATCH --partition=n1s8-v100-1
#SBATCH --account=bmsc_ga_4493

module purge

singularity exec --nv \
--bind /home,/scratch,/share/apps,/mnt \
--overlay /scratch/$USER/DL4Med/DL4Med_pytorch.ext3:ro \
--overlay /scratch/$USER/DL4Med/Project/images.sqf:ro \
/share/apps/images/cuda11.3.0-cudnn8-devel-ubuntu20.04.sif \
/bin/bash -c 'source /ext3/env.sh; python /scratch/$USER/DL4Med/Project/model.py'
```

1. Users need to login to Greene cluster first, instructions are available from Accessing HPC

2. From one greene login node, run

   ssh burst

3. On log-burst node, launch a simple CPU only interactive job for 4 hours

   srun --account=bmsc_ga_4493-2023sp --partition=interactive --time=04:00:00 --pty /bin/bash

4. A GPU job with 1 V100 GPU for 4 hours

   srun --account=bmsc_ga_4493-2023sp --partition=n1s8-v100-1 --gres=gpu:v100:1 --time=04:00:00 --pty /bin/bash

5. We are running spot instances on Cloud, instances could be shutdown by Google,

https://cloud.google.com/compute/docs/instances/spot
https://cloud.google.com/compute/docs/instances/preemptible

6. Please enable checkpoint/restart files for production runs, dump sheckpoint/restart file to **/scratch/NetID** folder

7. Please enable requeue for Slurm, jobs will be requeued automatically if the nodes are shutdown by GCP, new jobs should start from checkpoint/restart files

   #SBATCH --requeue

8. Greene Data transfer nodes is available with hostname **greene-dtn**. On a Cloud instances, run scp

scp -rp greene-dtn:/scratch/work/public/singularity/ubuntu-20.04.3.sif .

9. Instructions to setup Conda enviorment with Singularity and overlay file - Singularity with Miniconda

10. Overlay file templates are available from **/share/apps/overlay-fs-ext3**

11. Singularity OS images are available from **/share/apps/images**