A Quick Guide to Using CIRCE with GPU Capabilities

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Overview

The purpose of this quick guide is to provide simple steps to use GPU capabilities on CIRCE research cluster. It is assumed that the reader is familiar with Linux Shell and Virtual Environments in Python.

USF CIRCE has provided nice tutorials. Before you start, please visit the following online tutorials. They provide very useful information.

https://wiki rc.usf.edu

https://wiki.rc.usf.edu/index.php/Connecting_To_CIRCE

https://wiki.rc.usf.edu/index.php/Guide_to_SLURM

https://wiki.rc.usf.edu/index.php/CIRCE_Hardware

Step 1: Request Access

You need to request access to CIRCE by emailing <u>rc-help@usf.edu</u>. The administrators will create an account for you such that you can use it to login to CIRCE cluster.

Step 2: Install X2Go

CIRCE supports a nice remote desktop tool. You do not need tools such as PuTTY to do so. You will not need to directly connect to CIRCE via SSH (while possible, it is discouraged). You can find the installation steps <u>here</u> on CIRCE resources. This page includes all the steps necessary to set up a connection via x2Go with your USF credentials.

Step 3: Run X2Go

Once you set up X2Go. In your Linux shell you can start X2Go by typing:

x2goclient

Step 4: Installing and Creating a Virtual Environment (Miniconda)

In your remote desktop open a Linux shell and start installing Miniconda as your virtual environment. There is plenty of documentations on how to install Miniconda. Here is one way:

- 1- cd \$HOME
- 2- wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linuxx86_64.sh
- 3- chmod +x Miniconda3-latest-Linux-x86_64.sh
- 4- /Miniconda3-latest-Linux-x86_64.sh

When the installer asks "Do you wish the installer to initialize Miniconda3 by running conda init?", please answer "yes"

To check if miniconda is installed you can log-out of CIRCE, then log back in using X2GO.

1- which conda pip

It should return something like the following: ~/miniconda3/bin/conda and ~/miniconda3/bin/pip

```
2- pip install --upgrade pip
```

```
3- conda update --all -y
```

4- conda install -y anaconda

Now you can create a virtual environment and activate it.

conda create -n "name_of_your_environment"

```
source activate <name_of_your_environment>
```

Once the environment is activated, you can install other libraries such as PyTorch or TensorFlow inside your environment. For those installations, please refer to the official sites of these libraries.

Step 5: Transferring Your Files (code and/or data) to CIRCE

Now you can transfer your files to CIRCE using SFTP.

```
sftp username@circe.rc.usf.edu
```

You will be asked for your account credentials for logging in. Once you login, you can check the remote working directory by pwd command. The path that the pwd command returns is where you can find your files after they are transferred to CIRCE. put <your_pythoncode.py>

This will transfer your file to CIRCE. However, to run the code, it needs to be moved to a special folder in the working nodes on CIRCE. These are the nodes that are dedicated to run the code and are equipped with GPUs.

To do this, you can use the remote desktop GUI to move your file (<your_pythoncode.py>) to the following path: /work_bgfs/<first letter of your account username>/<your account username>

Tip: If your code requires data to run, you can transfer the data to CIRCE as described above and move the data in the same working directory as well.

Step 6: Running your Code on CIRCE

CIRCE provides an interactive shell environment in which you can run your code as you do on a local machine. To get to this environment you can run the following command.

```
srun --partition=muma_2021 -qos=muma21 --gres=gpu:1 --mem=10G -
time=03:00:00 --pty /bin/bash
```

Tip: The above command allocates the resource up to 3 hours. If your code takes more to run, please increase the time accordingly.

Now in this environment you can run you code simply after loading some modules to indicate your code needs to use GPU.

- 1- cd /work_bgfs/<first letter of your account username>/<your account username>
- 2- module load apps/cuda/12.2.2
- 3- source activate <name_of_your_environment>
- 4- python <your_pythoncode.py>

For questions you can always directly email <u>rc-help@usf.edu</u>.