GPU MINI-CLUSTER @RGNC

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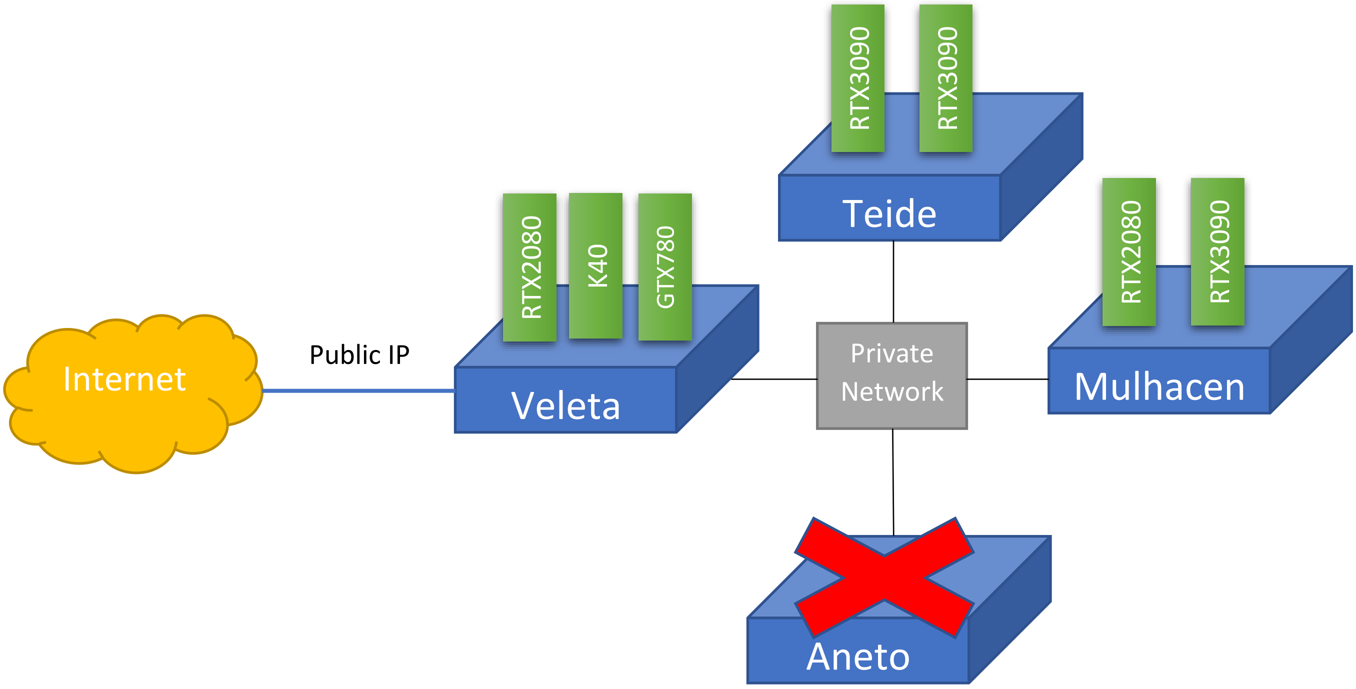
0. Contents

1. Description

Our mini-cluster is located at the Higher Technical School of Computer Engineering facilities, next to our Department of Computer Science and Artificial Intelligence. It is currently composed of **4** servers, named after the highest peaks of Spain: Teide (3715m, Canary Islands), Mulhacen (3479m, Granada), Aneto (3404m, Huesca), Veleta (3396m, Granada). The specifications are detailed at http://www.gcn.us.es/gpu_computing_servers. This is a picture of the servers taken in May 2022:

The configuration is the following:

- **Veleta** server can be openly accessed through a public IP of the university of Seville (we can give you the *IP if you collaborate with u*s, and you should have received it in the email with the credentials). It has three GPUs, two of them no longer supported in CUDA 12, so it will remains with CUDA 11.
- **Aneto** server is hidden behind Veleta server in a private network. Unfortunately, this server has hardware issues and it is unavailable.
- **Mulhacen** server is hidden behind Veleta server in a private network. It has two GPUs.
- **Teide** server is hidden behind Veleta server in a private network. It has two GPUs.



2. Client configuration

If you want to access each node by its name from your computer, do the following.

You should have Openssh Client in your operating system (e.g. in Ubuntu do `sudo apt install openssh-client`, in Windows install Openssh Client feature, etc.). You should have a folder `$HOME/.ssh` in your home directory (in your computer). If not, please create it: `mkdir $HOME/.ssh`. Next, backup your `$HOME/.ssh/config` file, if it exists already, by executing: `cp $HOME/.ssh/config $HOME/.ssh/config.backup`. If it doesn't exist, just continue with the next steps.

Next, download the config file from these links (depending on your operating system): linux or windows. Copy the file to your `$HOME/.ssh` folder.

Please, edit the `$HOME/.ssh/config` file with your favourite editor, and replace **GPU-RGNC** by the public IP of our server, and **USER** by the username given to you in the mini-cluster (you should have received by email). Also delete the comment (text after #) in those two lines (third and fourth line in the example below). At the end, you should have something like this (for example):

```
### First jumphost. Directly reachable
Host veleta
        HostName someservername.cs.us.es
        User gheorghepaun
        ProxyCommand none
        ForwardAgent yes
        GSSAPIAuthentication no

### Host to jump to via veleta
Host aneto
        HostName aneto
        ProxyCommand ssh veleta -W %h:%p
        ForwardAgent yes
        GSSAPIAuthentication no

### Host to jump to via veleta
Host mulhacen
        HostName mulhacen
        ProxyCommand ssh veleta -W %h:%p
        ForwardAgent yes
        GSSAPIAuthentication no

### Host to jump to via veleta
Host teide
        HostName teide
        ProxyCommand ssh veleta -W %h:%p
        ForwardAgent yes
        GSSAPIAuthentication no
```

If you don’t want to enter your password twice when accessing Teide, Mulhacen or Aneto through Veleta, execute the following lines in your machine (replace **USER** by your username given in the mini-cluster):

1. `ssh-keygen -t rsa -b 2048` (press enter for all the prompted questions)
2. `ssh-copy-id USER@aneto` (insert your password all the required times)
3. `ssh-copy-id USER@mulhacen` (insert your password all the required times)
4. `ssh-copy-id USER@teide` (insert your password all the required times)

Try for example "ssh **USER**@mulhacen", and check that you are requested only once for your password.

3. Access

If you have configured your ssh client as in previous section, you can access to each node independently. So, depending on the server (replace **USER** by your username in the mini-cluster):

- Access to Veleta: `ssh USER@veleta`
- Access to Aneto: `ssh USER@aneto`
- Access to Teide: `ssh USER@teide`
- Access to Mulhacen: `ssh USER@mulhacen`

Once you have accessed to the desired server, you can run your programs remotely. If you need to copy files to and from the servers, do the following (replace **USER** by your username and **NODE** by your desired node, either veleta, aneto, mulhacen or teide):

- Copy to a NODE: `scp YOUR_FILE USER@NODE:`
- Copy from a NODE: `scp USER@NODE:YOUR_FILE .`
- Copy a folder to a NODE: `scp -r YOUR_FOLDER USER@NODE:`
- Copy a folder from a NODE: `scp -r USER@NODE:YOUR_FOLDER .`

Please, keep using the password that you were given, or change it by another secure password. Do not use the password same as your username, or this kind of bad practices, since we are receiving lot of external attacks. In order to change the password, please execute `passwd` in each server (we don’t have a centralized user directory for the moment).

4. Working in a node

4.1 Book a time slot for your work

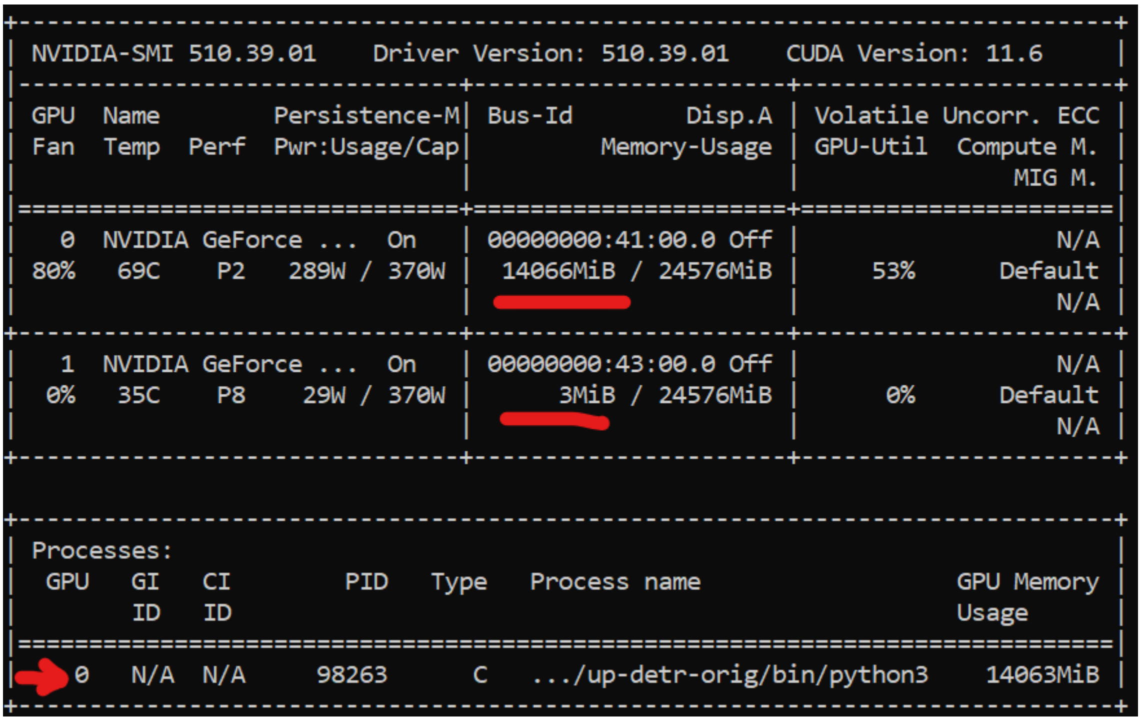
Given the high demand we have for our GPUs, please select a time slot here and book a GPU (or GPUs) for you. It is super-easy, just go to a GPU that you have access to, go to the day (row) and time (column) of your desire, and write your username to the hours you plan to use it. Please, be responsible and do not reserve the GPUs more than you expect to need (e.g. no more than two days in a row). Moreover, do not delete a reservation made by other user. We trust on the good behaviour of the users. In case you are having problems with other users, please notify to mdelamor ‘at’ us.es with the subject: [GPU at RGNC] USER REPORT, and explain the situation.

This is a temporary solution while we have a high demand, it can be replaced in the future with SLURM, tensorhive or something similar. Moreover, bear in mind that the RGNC can lock GPUs for research purposes. Required management time will be shown in the spreadsheet well in advance.

You do not need to reserve a GPU is your work is CPU only, e.g.: compilation, coding development, scripting, python and DL with CPU only, etc.

4.2 Selecting your GPU

Once you are logged in a node, you can check which GPUs are available and their status typing: `nvidia-smi`. Please, double check that your booked GPU is idle. The outcome of the instruction should be something as follows:



```
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 510.39.01    Driver Version: 510.39.01    CUDA Version: 11.6     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  NVIDIA GeForce ...  On   | 00000000:41:00.0 Off |                  N/A |
| 80%   69C    P2   289W / 370W |  14066MiB / 24576MiB |     53%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+
|   1  NVIDIA GeForce ...  On   | 00000000:43:00.0 Off |                  N/A |
|  0%   35C    P8    29W / 370W |      3MiB / 24576MiB |      0%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|    0   N/A  N/A     98263      C   .../up-detr-orig/bin/python3    14063MiB |
+-----------------------------------------------------------------------------+
```

In the example above, the first GPU is busy and 14GB is being used, while the GPU 1 is idle. You can see at the bottom of the output the processes using the GPUs. In the example, only one process is using GPU 0. In theory you can launch more than one process to the same GPU, as long as they fit in the memory. In any case, please try to avoid it, since the GPUs can be used for benchmarking, and this can affect performance.

By default you are given GPU number 0. In order to select a different GPU, or you want to use GPU number 1, type: `export CUDA_VISIBLE_DEVICES=1`. If you want to use both GPUs, type: `export CUDA_VISIBLE_DEVICES=0,1`. If you want to use GPU number 0 again, type: `export CUDA_VISIBLE_DEVICES=0`

4.3 Storage

All servers should have enough storage for your needs, but please check that home or / is not full by executing `df -h`. If you are using a large dataset, or you have lot of data, please consider moving it to the `/data` partition (Veleta, Mulhacen and Teide only). This partition has lot of space (1TB in Mulhacen and 2TB in Teide, Veleta has no such partition yet).

4.3 Selecting your compiler / development kit

We use **CVMFS** in all nodes for accessing different compilers and libraries versions. This is a CERN virtual file system with lot of development tools compiled for Red Hat based systems (CentOS, RockyLinux, AlmaLinux…). All our servers run Rocky Linux 9. In order to use cvmfs, do the following:

1. `ls /cvmfs/sft.cern.ch/lcg/releases` (this will mount the remote file system, and you will see all tools available, it is a long list)
2. For instance, if you want to use another version of *gcc* than the default one, select your version:
   - First, execute `ls /cvmfs/sft.cern.ch/lcg/releases/gcc` to see all available versions.
   - Select a version with a subfolder with centos9 (although centos7 usually works good as well).
   - For example, assume you want to use GCC 11.3.1, then just type: `source /cvmfs/sft.cern.ch/lcg/releases/gcc/11.3.1/x86_64-centos9/setup.sh`
3. Some other libraries instead of requiring a source file, just need to adjust your $PATH or your $LD_LIBRARY_PATH to that folder (for example for cmake)

You can check which are the available CUDA versions installed by running `ls -l /usr/local`.

We recommend using CVMFS for development, and python pip or conda for Machine Learning. If you need other software to get installed, and admin credentials are need, please email to mdelamor ‘at’ us.es with the subject [GPU at RGNC] SOFTWARE INSTALL.

4.3 Launching Jupyter Notebook for Python/Deep Learning

Both Jupyter Notebook and Lab are installed in all nodes. If you need to execute a remote **Jupyter notebook** environment, then do the following (replace **USER** by your username and **NODE** by your desired node, either veleta, aneto, mulhacen or teide):

1. Type in your machine: `ssh -L 8888:localhost:8888 USER@NODE`
2. In the node you chose, type:
   `jupyter notebook --port=8888 --no-browser`
   Copy the URL with the token shown at the end.
3. Now in your browser, paste the URL you copied before.

You may need to install jupyter by: *pip3 install jupyter*. If more than one user is using Jupyter notebook in the same server, **please change your port** in the lines above (e.g. 8889, 8890, 8891, etc.). Finally, anaconda is installed in our severs (though the `conda` command), in case you need to install a custom configuration. Please keep it at minimum since the disk space is limited, so consider using *miniconda* instead.

4.4 Remote development with NVIDIA Nsight Visual Studio Code

It is possible to use Remote Explorer plugin of NVIDIA Nsight Visual Studio in our servers. You will need to configure .ssh/config file from your active terminal in Visual Studio Code, as explained above. In this way, Visual Studio Code will find our servers.

4.5 Remote development with NVIDIA Nsight (deprecated)

You can use the remote application development in NVIDIA Nsight since version 6.5. More info: http://devblogs.nvidia.com/parallelforall/remote-application-development-nvidia-nsight-eclipse-edition/

There is no problem if you want to use our servers for remote application development. However, for Aneto, Mulhacen and Teide you have to do some extra work, since it cannot be seen by Nsight. A workaround for this is to do the following (replace USER by your username and NODE by your desired node Aneto, Mulhacen or Teide):

- In Nsight, go to properties of the project, Build → Target Systems.
- Select Manage..., and Add a new server
- Configure the new server as follows:
  - Host name: localhost
  - User name: *USER*
  - Label: *NODE*
  - System type: ssh, port: 9999
- Once you have that, just do the following in a Terminal before accessing the server via Nsight:
  - To run and profile an application, type:
    ```
    ssh -L 9999:localhost:22 USER@NODE
    ```
  - To debug an application (if you have configured port 2345 for the debugger), type:
    ```
    ssh -L 2345:localhost:2345 USER@NODE
    ```

Have fun, and wish you an efficient code!