GPU and Virtual Environment Instruction

Virtual Environment

Virtual environment allows group members to share a uniform Python environment. This means that when the virtual environment owner installs Python modules (i.e. specific version), it will also be available to other members who log into the environment. When group members want to work on a coding task, it is recommended to always enable virtual environment.

Procedure to Enter into a Virtual Environment:

1. SSH into an Imperial machine or use a lab computer using the command `ssh ic_username@machine_name.doc.ic.ac.uk` *(ic_username is your Imperial username and machine_name is machine name such as shell1, gpu11, etc)*
2. Access virtual environment using the command `source /vol/bitbucket/fm1710/venv/bin/activate`
3. Work on your group project
4. If you want to get out of the virtual environment, enter the command `deactivate`

GPU

GPU can be used to accelerate specific tasks that required parallel computations. Note that you don't submit your Python file to GPU, but instead you will first store your files inside `/vol/bitbucket/your_directory` and submit a job to the GPU cluster. For more information about this, see below.

Procedure to Submit a Job to GPU Cluster:

1. First create **your** own folder inside `/vol/bitbucket/` using the command `mkdir -p /vol/bitbucket/folder_name`. This folder serves as temporary file storage (Python, data, shell script) for jobs that will be submitted to the GPU *(folder_name is your folder name up to the user)*
2. Go inside your folder using `cd/vol/bitbucket/folder_name` and paste all necessary python files, data files, etc.
3. Create a `.sh` file which basically contains job instructions. Example of shell file (when we want the GPU to run `test1.py` and `test2.py`):

```
#!/bin/sh

# Run Python Files
python test1.py
python test2.py
```

4. Remotely access the cluster using the command `ssh gpucluster.doc.ic.ac.uk`
5. Enter virtual environment using command described above
6. Type the command `sbatch /vol/bitbucket/folder_name/shell_file_name` to run the job *(shell_file_name is `.sh` file that have been previously created)*

7. Then the output file will be produced inside your `/vol/bitbucket/folder_name/` directory with the `.out` extension.