How do I install PyTorch and TensorFlow with Python to use ccln2p3 GPU?

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- PyTorch and TensorFlow available without GPU
- How I did -> Probably not the best way to do
- For people who want to start quickly
- PyTorch 1.0.1.post2 and TensorFlow 1.13.0 (latest version on 28/03/2019)

Outline

- Requirements
  - Python version
  - Cuda version
- Installation
- Use
- Application example

Requirements - Python

- Python versions available at ccIn2p3

```
/pbs/software/centos-7-x86_64/python(0)>ll
total 394
drwxrwxr-x 9 dbouvet ccin2p3  163 11 avril   2018 2.7.14
drwxrwxr-x 9 dbouvet ccin2p3  163  4 juin    2018 2.7.15
drwxr-xr-x 8 dbouvet ccin2p3  142  5 oct.   17:22 2.7.3
drwxrwxr-x 9 gadrat  ccin2p3  163 26 sept.   2018 3.4.8
drwxrwxr-x 9 gadrat  ccin2p3  163 26 sept.   2018 3.6.5
drwxr-xr-x 9 gadrat  ccin2p3  163  5 déc.   10:45 3.6.7
-rwxrwxr-x 1 dbouvet ccin2p3  331 20 sept.   2018 ccenv.csh
-rwxrwxr-x 1 gadrat  ccin2p3  230 20 sept.   2018 ccenv.sh
-rw-rw-r-- 1 gadrat  ccin2p3   40 20 août    2018 ccenv.yaml
drwxr-xr-x 4 gadrat  ccin2p3   79  4 mars   13:28 modules
-rw-rw-r-- 1 gadrat  ccin2p3 2853 19 févr.  15:52 VERSIONS
```

- Mandatory versions

PyTorch   https://pytorch.org/get-started/locally/

PyTorch Build	Stable (1.0)		Preview (Nightly)	
Your OS	Linux	Mac		Windows
Package	Conda	Pip	LibTorch	Source
Language	Python 2.7	Python 3.5	Python 3.6	Python 3.7	C++
CUDA	8.0	9.0	10.0	None	
Run this Command:	pip3 install https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl pip3 install torchvision			

https://www.tensorflow.org/install/pip?lang=python3

✓ Python 3   Python 2.7

Check if your Python environment is already configured:

★ Requires Python 3.4, 3.5, or 3.6

Requirements - Python

- Change python version

```
/pbs/software/centos-7-x86_64/python(0)>cat ~/.profile | grep python -A 3
. python_env.sh 3.6.5
export LC_ALL=fr_FR.utf-8
export LANG=fr_FR.utf-8
```

- Creation of virtual environment

```
/pbs/throng/creatis/users/tbaudier(0)>cd
/pbs/home/t/tbaudier(0)>
/pbs/home/t/tbaudier(0)>
/pbs/home/t/tbaudier(0)>cd /pbs/throng/creatis/users/tbaudier/
/pbs/throng/creatis/users/tbaudier(0)>mkdir venvAI
/pbs/throng/creatis/users/tbaudier(0)>. python_env.sh 3.6.7
You are using version 3.6.7 of python.
/pbs/throng/creatis/users/tbaudier(0)>pip install --user virtualenv
Collecting virtualenv
  Using cached https://files.pythonhosted.org/packages/33/5d/314c760d4204f64e4a968275182b7751bd5c3249094757b39ba987dcfb5a/virtualenv-16.4.3-py2.py3-none-any.whl
Installing collected packages: virtualenv
  The script virtualenv is installed in '/pbs/home/t/tbaudier/.local/bin' which is not on PATH.
  Consider adding this directory to PATH or, if you prefer to suppress this warning, use --no-warn-script-location.
Successfully installed virtualenv-16.4.3
You are using pip version 19.0.2, however version 19.0.3 is available.
You should consider upgrading via the 'pip install --upgrade pip' command.
/pbs/throng/creatis/users/tbaudier(0)>virtualenv venvAI/
Using base prefix '/pbs/software/centos-7-x86_64/python/3.6.7'
New python executable in /pbs/throng/creatis/users/tbaudier/venvAI/bin/python3.6
Also creating executable in /pbs/throng/creatis/users/tbaudier/venvAI/bin/python
Installing setuptools, pip, wheel...
done.
/pbs/throng/creatis/users/tbaudier(0)>
```

Requirements - Cuda

- Connect to interactive GPU jobs

```
/pbs/home/t/tbaudier(0)>qlogin -l GPU=1 -l GPUtype=K80 -q mc_gpu_interactive -pe multicores_gpu 4
JSV "/opt/sge/util/resources/jsv/corebinding.jsv" has been started
JSV "/opt/sge/util/resources/jsv/corebinding.jsv" has been stopped
Your job 2206803 ("QLOGIN") has been submitted
waiting for interactive job to be scheduled ...
Your interactive job 2206803 has been successfully scheduled.
Establishing /usr/bin/qlogin_wrapper session to host ccwgige010.in2p3.fr ...
The authenticity of host '[ccwgige010.in2p3.fr]:41865 ([134.158.48.126]:41865)' can't be established.
ECDSA key fingerprint is SHA256:wmXwcX0cJrRE/D5kyxYRVq2hYpF7PTYHud6X4/Ygmh0.
ECDSA key fingerprint is MD5:93:0b:6c:35:dc:cd:6f:eb:9b:39:68:03:44:d7:a5:dc.
Are you sure you want to continue connecting (yes/no)? yes
Warning: Permanently added '[ccwgige010.in2p3.fr]:41865,[134.158.48.126]:41865' (ECDSA) to the list of known hosts.
tbaudier@ccwgige010.in2p3.fr's password:
Last login: Thu Mar 28 10:10:16 2019 from cca004.in2p3.fr

   ___  ___     __  __ _  ____  ____  ____
  / __)/ __)___(  )(  ( \(___ \(  _ \(  __ \
 ( (__( (__(___))( /    / / __/ ) __/ (__ (
  \___)\___)   (__)\_)__)(____)(__)  (____/

Platform: CentOS 7.6.1810
Architecture: x86_64


You are using version 3.6.5 of python.
[tbaudier@ccwgige010 ~]$ 
```

Requirements - Cuda

- Cuda versions available at ccIn2p3

```
[tbaudier@ccwgige010 ~]$ ll -d /opt/cuda-*
drwxr-xr-x 11 root root 4096  8 mars  14:07 /opt/cuda-10.1
drwxr-xr-x  3 root root   20 18 sept.  2018 /opt/cuda-7.5
drwxr-xr-x 11 root root 4096 26 sept.  2017 /opt/cuda-8.0
drwxr-xr-x 12 root root 4096 15 oct.  17:31 /opt/cuda-9.2
```

- Mandatory versions

https://pytorch.org/get-started/locally/

PyTorch Build	Stable (1.0)	Preview (Nightly)	
Your OS	Linux	Mac	Windows
Package	Conda	Pip	LibTorch	Source
Language	Python 2.7	Python 3.5	Python 3.6	Python 3.7	C++
CUDA	8.0	9.0	10.0	None
Run this Command:	pip3 install https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl pip3 install torchvision		

https://www.tensorflow.org/install/source

Version	Python version	Compiler	Build tools	cuDNN	CUDA
tensorflow_gpu-1.13.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.19.2	7.4	10.0
tensorflow_gpu-1.12.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.15.0	7	9
tensorflow_gpu-1.11.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.15.0	7	9
tensorflow_gpu-1.10.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.15.0	7	9
tensorflow_gpu-1.9.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.11.0	7	9
tensorflow_gpu-1.8.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.10.0	7	9
tensorflow_gpu-1.7.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.9.0	7	9
tensorflow_gpu-1.6.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.9.0	7	9
tensorflow_gpu-1.5.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.8.0	7	9
tensorflow_gpu-1.4.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.5.4	6	8
tensorflow_gpu-1.3.0	2.7, 3.3-3.6	GCC 4.8	Bazel 0.4.5	6	8

Requirements - Cuda

- Download and install Cuda 10.0

https://developer.nvidia.com/cuda-10.0-download-archive

Requirements - Cuda

- Download and install Cuda 10.0 - in an interactive GPU job

```
[tbaudier@ccwgige010 ~]$ cd /pbs/throng/creatis/users/tbaudier/
[tbaudier@ccwgige010 tbaudier]$ mkdir cuda100
[tbaudier@ccwgige010 tbaudier]$ cd cuda100/
[tbaudier@ccwgige010 cuda100]$ wget https://developer.nvidia.com/compute/cuda/10.0/Prod/local_installers/cuda_10.0.130_410.48_linux
--2019-03-28 14:54:53--  https://developer.nvidia.com/compute/cuda/10.0/Prod/local_installers/cuda_10.0.130_410.48_linux
Résolution de developer.nvidia.com (developer.nvidia.com)... 192.229.182.215
Connexion vers developer.nvidia.com (developer.nvidia.com)|192.229.182.215|:443...connecté.
requête HTTP transmise, en attente de la réponse...302 Found
Emplacement: https://developer.download.nvidia.com/compute/cuda/10.0/secure/Prod/local_installers/cuda_10.0.130_410.48_linux.run?8af_
iNNaU_o7b6HV6EnMCIj9BUxyPLjy9DV9rdyTLrZ3FzxgZoRDEtBXPy6PEOXGDgXJTvS6hUyLSyrvEVcdmq4WkYuM1_b6BAFXa0Vi1L6hs [suivant]
--2019-03-28 14:54:54--  https://developer.download.nvidia.com/compute/cuda/10.0/secure/Prod/local_installers/cuda_10.0.130_410.48_li
q5bLa-6KEN-CiNNaU_o7b6HV6EnMCIj9BUxyPLjy9DV9rdyTLrZ3FzxgZoRDEtBXPy6PEOXGDgXJTvS6hUyLSyrvEVcdmq4WkYuM1_b6BAFXa0Vi1L6hs
Résolution de developer.download.nvidia.com (developer.download.nvidia.com)... 192.229.221.58, 2606:2800:233:ef6:15dd:1ece:1d50:1e1
Connexion vers developer.download.nvidia.com (developer.download.nvidia.com)|192.229.221.58|:443...connecté.
requête HTTP transmise, en attente de la réponse...200 OK
Longueur: 2020126691 (1,9G) [application/octet-stream]
Sauvegarde en : «cuda_10.0.130_410.48_linux»

100%[====================================================================================================>============

2019-03-28 14:55:27 (76,1 MB/s) - «cuda_10.0.130_410.48_linux» sauvegardé [2020126691/2020126691]

[tbaudier@ccwgige010 cuda100]$ sh cuda_10.0.130_410.48_linux
Extraction failed.
Ensure there is enough space in /tmp and that the installation package is not corrupt
Signal caught, cleaning up
[tbaudier@ccwgige010 cuda100]$ □
```

Requirements - Cuda

- Download and install Cuda 10.0 - in an interactive GPU job

```
[tbaudier@ccwgige010 ~]$ cd /pbs/throng/creatis/users/tbaudier/
[tbaudier@ccwgige010 tbaudier]$ mkdir cuda100
[tbaudier@ccwgige010 tbaudier]$ cd cuda100/
[tbaudier@ccwgige010 cuda100]$ wget https://developer.nvidia.com/compute/cuda/10.0/Prod/local_installers/cuda_10.0.130_410.48_linux
--2019-03-28 14:54:53--  https://developer.nvidia.com/compute/cuda/10.0/Prod/local_installers/cuda_10.0.130_410.48_linux
Résolution de developer.nvidia.com (developer.nvidia.com)... 192.229.182.215
Connexion vers developer.nvidia.com (developer.nvidia.com)|192.229.182.215|:443...connecté.
requête HTTP transmise, en attente de la réponse...302 Found
Emplacement: https://developer.download.nvidia.com/compute/cuda/10.0/secure/Prod/local_installers/cuda_10.0.130_410.48_linux.run?8af_
iNNaU_o7b6HV6EnMCIj9BUxyPLjy9DV9rdyTLrZ3FzxgZoRDEtBXPy6PEOXGDgXJTvS6hUyLSyrvEVcdmq4WkYuM1_b6BAFXa0Vi1L6hs [suivant]
--2019-03-28 14:54:54--  https://developer.download.nvidia.com/compute/cuda/10.0/secure/Prod/local_installers/cuda_10.0.130_410.48_li
q5bLa-6KEN-CiNNaU_o7b6HV6EnMCIj9BUxyPLjy9DV9rdyTLrZ3FzxgZoRDEtBXPy6PEOXGDgXJTvS6hUyLSyrvEVcdmq4WkYuM1_b6BAFXa0Vi1L6hs
Résolution de developer.download.nvidia.com (developer.download.nvidia.com)... 192.229.221.58, 2606:2800:233:ef6:15dd:1ece:1d50:1e1
Connexion vers developer.download.nvidia.com (developer.download.nvidia.com)|192.229.221.58|:443...connecté.
requête HTTP transmise, en attente de la réponse...200 OK
Longueur: 2020126691 (1,9G) [application/octet-stream]
Sauvegarde en : «cuda_10.0.130_410.48_linux»

100%[==================================================================================================>]

2019-03-28 14:55:27 (76,1 MB/s) - «cuda_10.0.130_410.48_linux» sauvegardé [2020126691/2020126691]

[tbaudier@ccwgige010 cuda100]$ sh cuda_10.0.130_410.48_linux
Extraction failed.
Ensure there is enough space in /tmp and that the installation package is not corrupt
Signal caught, cleaning up
[tbaudier@ccwgige010 cuda100]$ 
```

ERROR

Requirements - Cuda

- Download and install Cuda 10.0 - without interactive job

```
/pbs/home/t/tbaudier(0)>cd /pbs/throng/creatis/users/tbaudier/
/pbs/throng/creatis/users/tbaudier(0)>mkdir cuda100
/pbs/throng/creatis/users/tbaudier(0)>cd cuda100/
/pbs/throng/creatis/users/tbaudier/cuda100(0)>wget https://developer.nvidia.com/compute/cuda/10.0/Prod/local_installers/cuda_10.0.130_410.48_linux
--2019-03-28 15:02:31--  https://developer.nvidia.com/compute/cuda/10.0/Prod/local_installers/cuda_10.0.130_410.48_linux
Résolution de developer.nvidia.com (developer.nvidia.com)... 192.229.182.215
Connexion vers developer.nvidia.com (developer.nvidia.com)|192.229.182.215|:443...connecté.
requête HTTP transmise, en attente de la réponse...302 Found
Emplacement: https://developer.download.nvidia.com/compute/cuda/10.0/secure/Prod/local_installers/cuda_10.0.130_410.48_linux.run?vtXso4kli0_mNlRLan
4C3rytUAPW9mujysdRcuCW_z9GVrcdrE9-XxKhCjKn2hSRgDhnpwvY9J-WMzAlRpx1frpPVaZgHKZaiegdoG3rQqyFj4e42Am7_xtnVIk [suivant]
--2019-03-28 15:02:32--  https://developer.download.nvidia.com/compute/cuda/10.0/secure/Prod/local_installers/cuda_10.0.130_410.48_linux.run?vtXso4k
w0X1dpkIpfSi4C3rytUAPW9mujysdRcuCW_z9GVrcdrE9-XxKhCjKn2hSRgDhnpwvY9J-WMzAlRpx1frpPVaZgHKZaiegdoG3rQqyFj4e42Am7_xtnVIk
Résolution de developer.download.nvidia.com (developer.download.nvidia.com)... 192.229.221.58, 2606:2800:233:ef6:15dd:1ece:1d50:1e1
Connexion vers developer.download.nvidia.com (developer.download.nvidia.com)|192.229.221.58|:443...connecté.
requête HTTP transmise, en attente de la réponse...200 OK
Longueur: 2020126691 (1,9G) [application/octet-stream]
Sauvegarde en : «cuda_10.0.130_410.48_linux»

100%[===============================================================================================================================
2019-03-28 15:02:47 (143 MB/s) - «cuda_10.0.130_410.48_linux» sauvegardé [2020126691/2020126691]

/pbs/throng/creatis/users/tbaudier/cuda100(0)>sh cuda_10.0.130_410.48_linux
```

Requirements - Cuda

- Download and install Cuda 10.0 - without interactive job

```
/pbs/throng/creatis/users/tbaudier/cuda100(0)>sh cuda_10.0.130_410.48_linux
Logging to /scratch/users/t/tbaudier/cuda_install_27619.log
Using less to view the EULA.
Do you accept the previously read EULA?
accept/decline/quit: accept

Install NVIDIA Accelerated Graphics Driver for Linux-x86_64 410.48?
(y)es/(n)o/(q)uit: no

Install the CUDA 10.0 Toolkit?
(y)es/(n)o/(q)uit: yes

Enter Toolkit Location
 [ default is /usr/local/cuda-10.0 ]: /pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0

Do you want to install a symbolic link at /usr/local/cuda?
(y)es/(n)o/(q)uit: no

Install the CUDA 10.0 Samples?
(y)es/(n)o/(q)uit: yes

Enter CUDA Samples Location
 [ default is /pbs/home/t/tbaudier ]: /pbs/throng/creatis/users/tbaudier/cuda100/

Installing the CUDA Toolkit in /pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0 ...
```

- Set environment variables

```
/pbs/home/t/tbaudier(0)>cat ~/.profile | grep "Cuda 10.0" -A 3
#Cuda 10.0 for pytorch & tensorflow
export PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/bin:${PATH}
export LD_LIBRARY_PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/lib64:${LD_LIBRARY_PATH}

/pbs/home/t/tbaudier(0)>
```

Installation

- Start interactive GPU jobs

```
/pbs/home/t/tbaudier(0)>qlogin -l GPU=1 -l GPUtype=K80 -q mc_gpu_interactive -pe multicores_gpu 4
```

- Set environment variables & start virtual environment

```
[tbaudier@ccwgige010 ~]$ . python_env.sh 3.6.7
You are using version 3.6.7 of python.
[tbaudier@ccwgige010 ~]$ export PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/bin:${PATH}
[tbaudier@ccwgige010 ~]$ export LD_LIBRARY_PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/lib64:${LD_LIBRARY_PATH}
[tbaudier@ccwgige010 ~]$ source /pbs/throng/creatis/users/tbaudier/venvAI/bin/activate
(venvAI) [tbaudier@ccwgige010 ~]$
(venvAI) [tbaudier@ccwgige010 ~]$ deactivate
[tbaudier@ccwgige010 ~]$ 
```

- Install PyTorch

```
(venvAI) [tbaudier@ccwgige010 ~]$ pip install https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl torchvision
Collecting torch==1.0.1.post2 from https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl
  Downloading https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl (636.8MB)
    100% |████████████████████████████| 636.8MB 15kB/s
Could not install packages due to an EnvironmentError: [Errno 28] Aucun espace disponible sur le périphérique
```

Installation

- ## Start interactive GPU jobs

```
/pbs/home/t/tbaudier(0)>qlogin -l GPU=1 -l GPUtype=K80 -q mc_gpu_interactive -pe multicores_gpu 4
```

- ## Set environment variables & start virtual environment

```
[tbaudier@ccwgige010 ~]$ . python_env.sh 3.6.7
You are using version 3.6.7 of python.
[tbaudier@ccwgige010 ~]$ export PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/bin:${PATH}
[tbaudier@ccwgige010 ~]$ export LD_LIBRARY_PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/lib64:${LD_LIBRARY_PATH}
[tbaudier@ccwgige010 ~]$ source /pbs/throng/creatis/users/tbaudier/venvAI/bin/activate
(venvAI) [tbaudier@ccwgige010 ~]$
(venvAI) [tbaudier@ccwgige010 ~]$ deactivate
[tbaudier@ccwgige010 ~]$ 
```

- ## Install PyTorch

```
(venvAI) [tbaudier@ccwgige010 ~]$ pip install https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl torchvision
Collecting torch==1.0.1.post2 from https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl
  Downloading https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl (636.8MB)
    100% |                                          | 636.8MB 15kB/s
Could not install packages due to an EnvironmentError: [Errno 28] Aucun espace disponible sur le périphérique
```

ERROR

Installation

- Set environment variables & start virtual environment

```
/pbs/home/t/tbaudier(0)>. python_env.sh 3.6.7
You are using version 3.6.7 of python.
/pbs/home/t/tbaudier(0)>export PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/bin:${PATH}
/pbs/home/t/tbaudier(0)>export LD_LIBRARY_PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/lib64:${LD_LIBRARY_PATH}
/pbs/home/t/tbaudier(0)>source /pbs/throng/creatis/users/tbaudier/venvAI/bin/activate
(venvAI) /pbs/home/t/tbaudier(0)>
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- Install PyTorch

○ PyTorch https://pytorch.org/get-started/locally/

PyTorch Build	Stable (1.0)		Preview (Nightly)	
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CUDA	8.0	9.0	10.0	None
Run this Command:	pip3 install https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl
pip3 install torchvision			

Installation

- Set environment variables & start virtual environment

```
/pbs/home/t/tbaudier(0)>. python_env.sh 3.6.7
You are using version 3.6.7 of python.
/pbs/home/t/tbaudier(0)>export PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/bin:${PATH}
/pbs/home/t/tbaudier(0)>export LD_LIBRARY_PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/lib64:${LD_LIBRARY_PATH}
/pbs/home/t/tbaudier(0)>source /pbs/throng/creatis/users/tbaudier/venvAI/bin/activate
(venvAI) /pbs/home/t/tbaudier(0)>
```

- Install PyTorch

```
(venvAI) /pbs/home/t/tbaudier(0)>pip install https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl torchvision
Collecting torch==1.0.1.post2 from https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl
  Using cached https://download.pytorch.org/whl/cu100/torch-1.0.1.post2-cp36-cp36m-linux_x86_64.whl
Collecting torchvision
  Downloading https://files.pythonhosted.org/packages/fb/01/03fd7e503c16b3dc262483e5555ad40974ab5da8b9879e164b56c1f4ef6f/torchvision-0.2.2.pos
    100% |████████████████████████████████| 71kB 1.7MB/s
Collecting pillow>=4.1.1 (from torchvision)
  Downloading https://files.pythonhosted.org/packages/85/5e/e91792f198bbc5a0d7d3055ad552bc4062942d27eaf75c3e2783cf64eae5/Pillow-5.4.1-cp36-cp3
    100% |████████████████████████████████| 2.0MB 1.8MB/s
Collecting six (from torchvision)
  Downloading https://files.pythonhosted.org/packages/73/fb/00a976f728d0d1fecfe898238ce23f502a721c0ac0ecfedb80e0d88c64e9/six-1.12.0-py2.py3-no
Collecting numpy (from torchvision)
  Downloading https://files.pythonhosted.org/packages/35/d5/4f8410ac303e690144f0a0603c4b8fd3b986feb2749c435f7cdbb288f17e/numpy-1.16.2-cp36-cp3
    100% |████████████████████████████████| 17.3MB 904kB/s
Installing collected packages: torch, pillow, six, numpy, torchvision
Successfully installed numpy-1.16.2 pillow-5.4.1 six-1.12.0 torch-1.0.1.post2 torchvision-0.2.2.post3
(venvAI) /pbs/home/t/tbaudier(0)>
```

Installation

- Install TensorFlow

```
(venvAI) /pbs/home/t/tbaudier(0)>pip install tensorflow tensorflow-gpu
Collecting tensorflow
  Using cached https://files.pythonhosted.org/packages/77/63/a9fa76de8dffe745530
Collecting tensorflow-gpu
  Using cached https://files.pythonhosted.org/packages/7b/b1/0ad4ae02e17ddd62109
Collecting tensorflow-estimator<1.14.0rc0,>=1.13.0 (from tensorflow)
  Downloading https://files.pythonhosted.org/packages/bb/48/13f49fc3fa0fdf916aa1
    100% |                                    | 368kB 2.3MB/s
Collecting grpcio>=1.8.6 (from tensorflow)
  Downloading https://files.pythonhosted.org/packages/f4/dc/5503d89e530988eb7a1a
    100% |                                    | 10.8MB 1.2MB/s
```

■ ■ ■

```
Collecting pbr>=0.11 (from mock>=2.0.0->tensorflow-estimator<1.14.0rc0,>=1.13.0-
>tensorflow)
  Downloading https://files.pythonhosted.org/packages/14/09/12fe9a14237a6b7e0ba3
a8d6fcf254bf4b10ec56a0185f73d651145e9222/pbr-5.1.3-py2.py3-none-any.whl (107kB)
    100% |                                    | 112kB 3.3MB/s
Building wheels for collected packages: gast, termcolor, absl-py
  Building wheel for gast (setup.py) ... done
  Stored in directory: /pbs/home/t/tbaudier/.cache/pip/wheels/5c/2e/7e/a1d4d4fce
be6c381f378ce7743a3ced3699feb89bcfbdadadd
  Building wheel for termcolor (setup.py) ... done
  Stored in directory: /pbs/home/t/tbaudier/.cache/pip/wheels/7c/06/54/bc84598ba
1daf8f970247f550b175aaaee85f68b4b0c5ab2c6
  Building wheel for absl-py (setup.py) ... done
  Stored in directory: /pbs/home/t/tbaudier/.cache/pip/wheels/ee/98/38/46cbcc5a9
3cfea5492d19c38562691ddb23b940176c14f7b48
Successfully built gast termcolor absl-py
Installing collected packages: absl-py, pbr, mock, tensorflow-estimator, grpcio,
 h5py, keras-applications, gast, termcolor, keras-preprocessing, protobuf, werkz
eug, markdown, tensorboard, astor, tensorflow, tensorflow-gpu
Successfully installed absl-py-0.7.1 astor-0.7.1 gast-0.2.2 grpcio-1.19.0 h5py-2
.9.0 keras-applications-1.0.7 keras-preprocessing-1.0.9 markdown-3.1 mock-2.0.0
pbr-5.1.3 protobuf-3.7.1 tensorboard-1.13.1 tensorflow-1.13.1 tensorflow-estimat
or-1.13.0 tensorflow-gpu-1.13.1 termcolor-1.1.0 werkzeug-0.15.1
(venvAI) /pbs/home/t/tbaudier(0)>
```

Installation

- Check installation

```
(venvAI) /pbs/home/t/tbaudier(1)>pip freeze
absl-py==0.7.1
astor==0.7.1
gast==0.2.2
grpcio==1.19.0
h5py==2.9.0
Keras-Applications==1.0.7
Keras-Preprocessing==1.0.9
Markdown==3.1
mock==2.0.0
numpy==1.16.2
pbr==5.1.3
Pillow==5.4.1
protobuf==3.7.1
six==1.12.0
tensorboard==1.13.1
tensorflow==1.13.1
tensorflow-estimator==1.13.0
tensorflow-gpu==1.13.1
termcolor==1.1.0
torch==1.0.1.post2
torchvision==0.2.2.post3
Werkzeug==0.15.1
(venvAI) /pbs/home/t/tbaudier(0)>
```

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Installation

- Check installation – in an interactive GPU job

```
/pbs/home/t/tbaudier(0)>qlogin -l GPU=1 -l GPUtype=K80 -q mc_gpu_interactive -pe multicores_gpu 4

[tbaudier@ccwgige010 ~]$ . python_env.sh 3.6.7
You are using version 3.6.7 of python.
[tbaudier@ccwgige010 ~]$ export PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/bin:${PATH}
[tbaudier@ccwgige010 ~]$ export LD_LIBRARY_PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/lib64:${LD_LIBRARY_PATH}
[tbaudier@ccwgige010 ~]$ source /pbs/throng/creatis/users/tbaudier/venvAI/bin/activate
(venvAI) [tbaudier@ccwgige010 ~]$
```

- Check PyTorch:

```
(venvAI) [tbaudier@ccwgige010 ~]$ python
Python 3.6.7 (default, Dec  5 2018, 09:50:29)
[GCC 4.8.5 20150623 (Red Hat 4.8.5-36)] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import torch
>>> torch.cuda.is_available()
True
>>> torch.cuda.get_device_name(0)
'Tesla K80'
>>> print(torch.rand(3,3).cuda())
tensor([[0.5956, 0.5658, 0.5196],
        [0.7455, 0.1029, 0.7484],
        [0.0840, 0.4392, 0.6628]], device='cuda:0')
>>> 
```

Installation

- ## Check TensorFlow:

```
(venvAI) [tbaudier@ccwgige010 ~]$ python
Python 3.6.7 (default, Dec  5 2018, 09:50:29)
[GCC 4.8.5 20150623 (Red Hat 4.8.5-36)] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow as tf
>>> tf.Session(config=tf.ConfigProto(log_device_placement=True))
2019-03-28 16:53:39.787518: I tensorflow/core/platform/cpu_feature_guard.cc:141] Your CPU supports instructions that this TensorFlow binary was not compiled to use: AVX2 FMA
2019-03-28 16:53:39.883653: I tensorflow/compiler/xla/service/service.cc:150] XLA service 0x43c9460 executing computations on platform CUDA. Devices:
2019-03-28 16:53:39.883699: I tensorflow/compiler/xla/service/service.cc:158]   StreamExecutor device (0): Tesla K80, Compute Capability 3.7
2019-03-28 16:53:39.885903: I tensorflow/core/platform/profile_utils/cpu_utils.cc:94] CPU Frequency: 2599805000 Hz
2019-03-28 16:53:39.886049: I tensorflow/compiler/xla/service/service.cc:150] XLA service 0x44308c0 executing computations on platform Host. Devices:
2019-03-28 16:53:39.886068: I tensorflow/compiler/xla/service/service.cc:158]   StreamExecutor device (0): <undefined>, <undefined>
2019-03-28 16:53:39.886779: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1433] Found device 0 with properties:
name: Tesla K80 major: 3 minor: 7 memoryClockRate(GHz): 0.8235
pciBusID: 0000:05:00.0
totalMemory: 11.17GiB freeMemory: 11.11GiB
2019-03-28 16:53:39.886807: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1512] Adding visible gpu devices: 0
2019-03-28 16:53:39.888456: I tensorflow/core/common_runtime/gpu/gpu_device.cc:984] Device interconnect StreamExecutor with strength 1 edge matrix:
2019-03-28 16:53:39.888471: I tensorflow/core/common_runtime/gpu/gpu_device.cc:990]      0
2019-03-28 16:53:39.888478: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1003] 0:   N
2019-03-28 16:53:39.889097: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1115] Created TensorFlow device (/job:localhost/replica:0/task:0/device:GPU:0 with 10805 MB memory)
: Tesla K80, pci bus id: 0000:05:00.0, compute capability: 3.7)
Device mapping:
/job:localhost/replica:0/task:0/device:XLA_GPU:0 -> device: XLA_GPU device
/job:localhost/replica:0/task:0/device:XLA_CPU:0 -> device: XLA_CPU device
/job:localhost/replica:0/task:0/device:GPU:0 -> device: 0, name: Tesla K80, pci bus id: 0000:05:00.0, compute capability: 3.7
2019-03-28 16:53:39.889718: I tensorflow/core/common_runtime/direct_session.cc:317] Device mapping:
/job:localhost/replica:0/task:0/device:XLA_GPU:0 -> device: XLA_GPU device
/job:localhost/replica:0/task:0/device:XLA_CPU:0 -> device: XLA_CPU device
/job:localhost/replica:0/task:0/device:GPU:0 -> device: 0, name: Tesla K80, pci bus id: 0000:05:00.0, compute capability: 3.7

<tensorflow.python.client.session.Session object at 0x2b41c68fdb00>
>>> 
```

Use

- Create ~/testAI.job:

```
# Correct path in sps
cd /sps/creatis/tbaudier/testAI/

# Set correct python
. python_env.sh 3.6.7
export LC_ALL=fr_FR.utf-8
export LANG=fr_FR.utf-8

# Set Cuda 10.0 environment variables
export PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/bin:${PATH}
export LD_LIBRARY_PATH=/pbs/throng/creatis/users/tbaudier/cuda100/cuda-10.0/lib64:${LD_LIBRARY_PATH}

# Start python virtual environment
source /pbs/throng/creatis/users/tbaudier/venvAI/bin/activate

which python

# Main part
python ./testAI.py

# Close virtual environment
deactivate
```

Use

- Create /sps/creatis/tbaudier/testAI/testAI.py:

```python
import torch
import tensorflow as tf

#Pytorch test
print(torch.cuda.is_available())
print(torch.cuda.get_device_name(0))
print(torch.rand(3,3).cuda())

#Tensorflow test
a = tf.constant([1.0, 2.0, 3.0, 4.0, 5.0, 6.0], shape=[2, 3], name='a')
b = tf.constant([1.0, 2.0, 3.0, 4.0, 5.0, 6.0], shape=[3, 2], name='b')
c = tf.matmul(a, b)
sess = tf.Session(config=tf.ConfigProto(log_device_placement=True))
print(sess.run(c))
```

Use

- Run GPU job:

```
/pbs/home/t/tbaudier(0)>qsub -l h_fsize=1G,s_cpu=1:00:00,h_rss=1G,GPU=1,GPUtype=V100 -pe multicores_gpu 4 testAI.job
Your job 2215873 ("testAI.job") has been submitted
```

- Output log:

```
/pbs/home/t/tbaudier(0)>cat testAI.job.o2215873
Cleared Accounted PIDs for GPU 00000000:AF:00.0.
All done.
***************************************************************
*                  Grid Engine Batch System                  *
*          IN2P3 Computing Centre, Villeurbanne FR            *
***************************************************************
* User:               tbaudier                               *
* Group:              creatis                                 *
* Jobname:            testAI.job                              *
* JobID:              2215873                                 *
* Queue:              mc_gpu_medium                           *
* Worker:             ccwgpge012.in2p3.fr                     *
* Operating system:   Linux 3.10.0-957.5.1.el7.x86_64         *
* Project:            P_creatis                               *
***************************************************************
* Submitted on:       jeu. mars 28 17:13:49 2019              *
* Started on:         jeu. mars 28 17:14:02 2019              *
***************************************************************

/pbs/throng/creatis/users/tbaudier/venvAI/bin/python
True
Tesla V100-PCIE-32GB
tensor([[0.3183, 0.6610, 0.1380],
        [0.6139, 0.6171, 0.4197],
        [0.4921, 0.9900, 0.3816]], device='cuda:0')
[[22. 28.]
 [49. 64.]]
Device mapping:
/job:localhost/replica:0/task:0/device:XLA_GPU:0 -> device: XLA_GPU device
/job:localhost/replica:0/task:0/device:XLA_CPU:0 -> device: XLA_CPU device
/job:localhost/replica:0/task:0/device:GPU:0 -> device: 0, name: Tesla V100-PCIE-32GB, pci bus id: 0000:af:00.0, compute capability: 7.0
MatMul: (MatMul): /job:localhost/replica:0/task:0/device:GPU:0
a: (Const): /job:localhost/replica:0/task:0/device:GPU:0
b: (Const): /job:localhost/replica:0/task:0/device:GPU:0
```

```
***************************************************************
* GPU requested: 1                                           *
***************************************************************
* TeslaV100-PCIE-32GB: GPU-a1275a52
*   time:               10317ms                              *
*   gpu_utilization:    1%                                   *
*   mem_utilization:    0%                                   *
*   max_memory_usage:   0MiB                                 *
# lines inserted: 1

***************************************************************
* Ended on:            jeu. mars 28 17:14:25 2019            *
* Exit status:         0                                     *
* Consumed                                                   *
*   cpu (HS06):         00:00:00                             *
*   cpu scaling factor: 17.770000                           *
*   cpu time:           0 / 14400                            *
*   efficiency:         00 %                                 *
*   io:                 0.00000GB                            *
*   vmem:               N/A                                  *
*   maxvmem:            N/A                                  *
*   maxrss:             N/A                                  *
+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

Application

- Monte-Carlo simulation in medical physics
  - For dose computation in radiation therapy
  - For nuclear imaging (SPECT, PET)

- Investigate the use of Neural Network in Variance Reduction Technique (VRT) to speed up simulation

- Current project: learn Phase-Space file (PHSP) with GAN
  - PHSP = 1e8 particles, E, x, y, z, dx, dy, dz, ~3 GB
  - GAN: Generative Adversarial Network
  - Output is ~3 MB
  - PyTorch
  - 1 job 1 GPU, 1h-5h according parameter numbers

Marginal distribution
Courtesy of David SARRUT