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Guide: OpenACC on AWS

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Abstract

This is a guideline document to show the necessary actions to set up the system to use **OpenACC** in **GPU-base accelerated computing instances on AWS**.

Requirements

- **First you should have followed the Guide “First Access to AWS”**. It is assumed you already have an AWS account and a key pair, and you are familiar with the AWS EC2 environment.
- Take into account that **GPU-powered instances are expensive**.

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1. Configure the VM

- Launch an instance with **"Ubuntu Server 18.04"** as AMI and **"g3.4xlarge"** as instance type. This is an instance powered by one NVIDIA Tesla M60 GPU with **8 GiB of GPU memory** and **2048 parallel processing cores**. [Your default account may not allow you to use any GPUs (including g3.4xlarge). In that case, via "support" on AWS dashboard, request access to **g3.4xlarge**.]
- You should include the internal hostname and IP to **/etc/hosts**. You will find these under Description once the instance is up and running. In my specific case:

```
$ cat /etc/hosts
127.0.0.1 localhost
172.30.4.157 ip-172-30-4-157
```

- Check the availability of the GPU within the running instance

```
$ lspci | grep -i nvidia

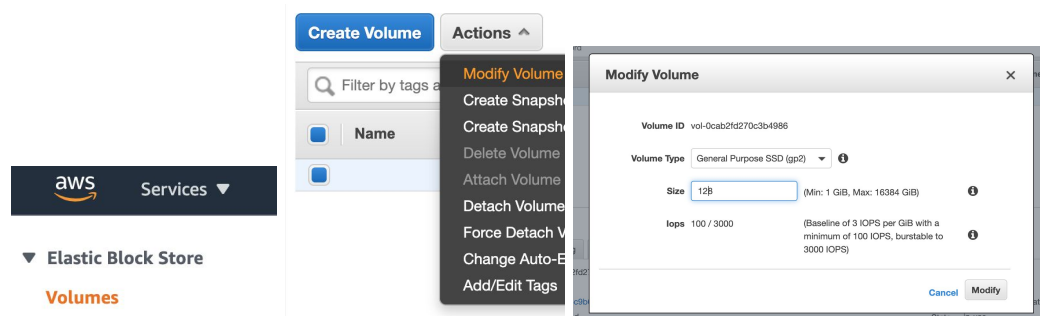
00:1e.0 VGA compatible controller: NVIDIA Corporation
GM204GL [Tesla M60] (rev a1)
```

- By default the **EBS volume is only 8GiB and we need 128GiB**.

```
$ df -h
```

Filesystem	Size	Used	Avail	Use%	Mounted on
udev	60G	0	60G	0%	/dev
tmpfs	12G	8.7M	12G	1%	/run
/dev/xvda1	8G	6G	4.0G	69%	/

- Go to the **AWS control panel** and in the **Volumes section** of the EC2 dashboard find your **EBS partition** and **resize its volume**.





- Then within the running system you have to **extend the Linux File System.**

```
$ sudo growpart /dev/xvda 1
```

```
CHANGED:  disk=/dev/xvda  partition=1:  start=4096  old:
size=16773086,end=16777182 new: size=73396190,end=73400286
```

- A look at the **lsblk** output confirms that the partition `/dev/xvda1` now fills the **available space on the volume** `/dev/xvda`:

```
$ lsblk
```

```
NAME      MAJ:MIN RM  SIZE RO TYPE MOUNTPOINT
...
xvda      202:80   0  128G  0 disk
└─xvda1   202:81   0  128G  0 part
```

- Use a file system-specific command to **resize each file system** to the new volume capacity. For a Linux ext2, ext3, or ext4 **file system**, use the following command, **substituting the device name to extend**:

```
$ sudo resize2fs /dev/xvda1
```

- Make sure we have some **basic packages installed on Ubuntu**

```
$ sudo apt-get update
```

```
$ sudo apt-get install build-essential
```

- The `gcc` version I'm using is 7.x

```
$ gcc --version
```

```
gcc (Ubuntu 7.5.0-3ubuntu1~18.04) 7.5.0
```

2. Install CUDA

- Use **wget** from the EC2 instance

```
$ wget
```

```
http://developer.download.nvidia.com/compute/cuda/repos/ubuntu1804/x86\_64/cuda-repo-ubuntu1804\_10.0.130-1\_amd64.deb
```



- We should now have a deb file called `cuda-repo-ubuntu1804_10.0.130-1_amd64.deb` in the home directory. Run the following commands to install CUDA:

```
$ sudo dpkg -i cuda-repo-ubuntu1804_10.0.130-1_amd64.deb
```

You may receive a “The public CUDA GPG key does not appear to be installed.” error. Please paste and run the command it recommends, which will look something like

```
$ sudo apt-key adv --fetch-keys
http://developer.download.nvidia.com/compute/cuda/repos/ubuntu1804/x86_64/7fa2af80.pub
```

- Continue your installation with the following commands:

```
$ sudo apt-get update
$ sudo apt-get install cuda
```

- Now you can check the CUDA installation:

```
$ nvidia-smi
```

```
Wed Feb 17 05:07:39 2021
```

```
+-----+
| NVIDIA-SMI 460.32.03      Driver Version: 460.32.03      CUDA Version: 11.2      |
+-----+-----+-----+-----+
| 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   Tesla M60                Off | 00000000:00:1E.0 Off |                    0 |
| N/A    28C    P0              38W / 150W |  0MiB /  7618MiB |      98%      Default |
|                                           | N/A           |
+-----+-----+-----+-----+
```

```
+-----+
| Processes:                                                                 |
|  GPU   GI    CI          PID    Type   Process name                      GPU Memory |
|          ID    ID                                   Usage                    |
+=====+=====+=====+=====+
| No running processes found                                              |
+-----+
```

- This command may take a few seconds to run due to the default configurations being suboptimal. You can follow the steps below to re-configure the GPU settings:

- Configure the GPU settings to be persistent

```
$ sudo nvidia-smi -pm 1
```

- Disable the autoboot feature for all GPUs on the instance

```
$ sudo nvidia-smi --auto-boost-default=0
```

- Set all GPU clock speeds to their maximum frequency

```
$ sudo nvidia-smi -ac 2505,875
```

- Running `nvidia-smi` may now be faster!

3. Install NVIDIA HPC SDK

The NVIDIA HPC SDK includes a no-cost license to a recent release of the Fortran, C and C++ compilers and tools for multicore CPUs and NVIDIA Tesla GPUs, including all OpenACC, OpenMP and CUDA Fortran features.

- Install NVIDIA HPC SDK Version 21.1 with the following

```
$ wget
https://developer.download.nvidia.com/hpc-sdk/21.1/nvhpc_2021
_211_Linux_x86_64_cuda_11.2.tar.gz

$ tar xpf nvhpc_2021_211_Linux_x86_64_cuda_11.2.tar.gz

$ sudo nvhpc_2021_211_Linux_x86_64_cuda_11.2/install
```

During install you will need to go through the following steps:

1. You will then be asked if you want to do a single system install or a network. Choose **1 for single system**
 2. Then you will be asked which directory you would like to install in. Press **enter** to keep the default `/opt/nvidia/hpc_sdk`
- Configure your shell environment.

```
$ export PGI=/opt/nvidia/hpc_sdk;
$ export
PATH=/opt/nvidia/hpc_sdk/Linux_x86_64/21.1/compilers/bin:$PATH;
$ export
MANPATH=$MANPATH:/opt/nvidia/hpc_sdk/Linux_x86_64/21.1/compiler
```



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s/man;

- Run `pgaccelinfo` to see that your GPU and drivers are properly installed and available. For NVIDIA, you should see output that looks something like the following:

```
$ pgaccelinfo
CUDA Driver Version:           11020
NVRM version:                  NVIDIA UNIX x86_64 Kernel Module
460.32.03   Sun Dec 27 19:00:34 UTC 2020

Device Number:                 0
Device Name:                   Tesla M60
Device Revision Number:        5.2
Global Memory Size:            7988903936
Number of Multiprocessors:      16
Concurrent Copy and Execution: Yes
Total Constant Memory:         65536
Total Shared Memory per Block: 49152
Registers per Block:           65536
Warp Size:                     32
Maximum Threads per Block:     1024
Maximum Block Dimensions:      1024, 1024, 64
Maximum Grid Dimensions:       2147483647 x 65535 x 65535
Maximum Memory Pitch:          2147483647B
Texture Alignment:             512B
Clock Rate:                     873 MHz
Execution Timeout:             No
Integrated Device:             No
Can Map Host Memory:          Yes
Compute Mode:                  default
Concurrent Kernels:           Yes
ECC Enabled:                   Yes
Memory Clock Rate:             2505 MHz
Memory Bus Width:              256 bits
L2 Cache Size:                 2097152 bytes
Max Threads Per SMP:           2048
Async Engines:                 2
Unified Addressing:            Yes
Managed Memory:               Yes
Concurrent Managed Memory:     No
Default Target:                cc50
```

4. Our First OpenACC Program

- Upload to the VM the [acc_sc.c](#) code, compile it with `pgcc`, and run the code on the GPU. Use

options `-acc` to support OpenACC and `-Minfo` to provide verbose info:

```
$ pgcc -acc -Minfo acc_sc.c -o acc_sc
```

vecaddgpu:

```
4, Generating copyin(a[:n])
   Generating copyout(r[:n])
   Generating copyin(b[:n])
5, Loop is parallelizable
   Accelerator kernel generated
   Generating Tesla code
5, #pragma acc loop gang, vector(128)/* blockIdx.x threadIdx.x */
```

- Run the code

```
$ ./acc_sc
```

- You should see the output

```
0 errors found
```

- You can enable additional output by setting environment variables.

```
$ export PGI_ACC_NOTIFY=1
```

- Run the code again and you should see the output

```
launch      CUDA      kernel      file=/home/ubuntu/acc_sc.c
function=vecaddgpu line=5 device=0 threadid=1 num_gangs=782
num_workers=1 vector_length=128 grid=782 block=128
```

```
0 errors found
```

- The extra output tells you that the program launched a kernel for the loop at line 5, with a CUDA grid of size 782, and a thread block of size 128.
- if you set the environment variable `PGI_ACC_NOTIFY` to 3, the output will include information about the data transfers as well:

```
upload CUDA data file=/home/ubuntu/acc_sc.c function=vecaddgpu
line=3 device=0 threadid=1 variable=a bytes=400000
```

```
upload CUDA data file=/home/ubuntu/acc_sc.c function=vecaddgpu
line=3 device=0 threadid=1 variable=b bytes=400000
```

```
launch      CUDA      kernel      file=/home/ubuntu/acc_sc.c
function=vecaddgpu line=5 device=0 threadid=1 num_gangs=782
num_workers=1 vector_length=128 grid=782 block=128
```



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```
download      CUDA      data      file=/home/ubuntu/acc_sc.c
function=vecaddgpu line=5 device=0 threadid=1 variable=r
bytes=400000

0 errors found
```

- If you **set the environment variable** `PGI_ACC_TIME to 1` (`export PGI_ACC_TIME=1`), the runtime summarizes the time taken for data movement between the host and GPU, and computation on the GPU.

Accelerator Kernel Timing data

/home/ubuntu/acc_sc.c

vecaddgpu NVIDIA devicenum=0

time(us): 149

3: compute region reached 1 time

5: kernel launched 1 time

grid: [782] block: [128]

device time(us): total=8 max=8 min=8 avg=8

elapsed time(us): total=679 max=679 min=679 avg=679

3: data region reached 2 times

3: data copyin transfers: 2

device time(us): total=93 max=51 min=42 avg=46

5: data copyout transfers: 1

device time(us): total=48 max=48 min=48 avg=48

- This tells you that the program **entered one accelerator region** and spent a total of about 149 microseconds in that region. It copied two arrays to the device, launched one kernel and brought one array back to the host.

Stop your instances when are done for the day to avoid



incurring charges
Terminate them when you are sure you are done with your
instance