INSTITUTE FOR APPLIED COMPUTATIONAL SCIENCE AT HARVARD UNIVERSITY

HARVARD School of Engineering and Applied Sciences

Guide: OpenACC on AWS

Ignacio M. Llorente, David Sondak, Simon Warchol

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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
```

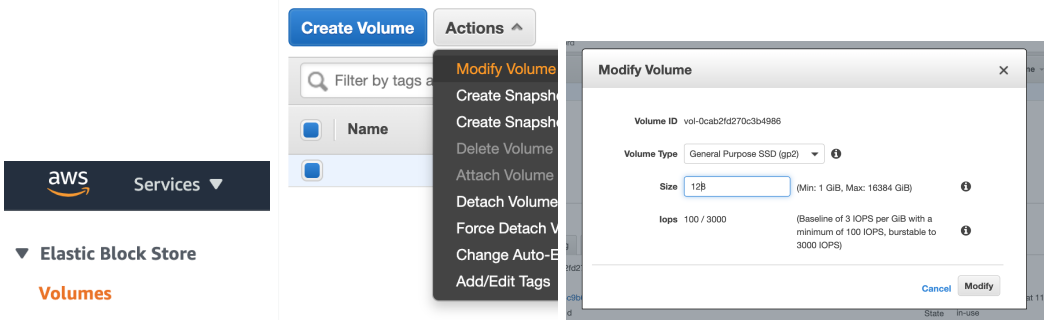
- Check the availability of the GPU within the running instance

```
$ 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/ubu
ntu1804/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 autoboost 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 xpzf 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
```

```
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
```

```
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