GPU Computing (CS 205)

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Odyssey and GPU Computing on Odyssey

Before proceeding further, make yourself familiar with the basics of Odyssey and GPU computing on Odyssey:
https://rc.fas.harvard.edu/resources/odyssey-quickstart-guide/
https://rc.fas.harvard.edu/resources/documentation/gpgpu-computing-on-odyssey/

CUDA

Compiling and running CUDA code

1) Login to a node with a GPU, eg. holyseasgpu (for CS 205)
   
   srun --pty --x11=first -p holyseasgpu --mem 4000 -t 0-5:00 -n 1 -N 1 /bin/bash

2) In a command window, type:
   
   source new-modules.sh
   module load cuda/7.5-fasrc01

If your cuda program is 'test.cu', then you can compile with:

   nvcc test.cu -o test

You can also use makefiles. Here is an example cuda code with a makefile:

   main.cu
   makefile

with these two files in the same directory, you can type, on the command line:

   make

This will produce an executable 'square'

3) Run the cuda executable with the runscript:

   #!/bin/bash
   #SBATCH -p holyseasgpu #Partition to submit to
   #SBATCH -n 1 #Number of cores
   #SBATCH --gres=gpu
   #SBATCH --time=5 #Runtime in minutes
   #SBATCH --mem-per-cpu=100 #Memory per cpu in MB (see also --mem)
   #SBATCH --constraint=cuda-7.5

   source new-modules.sh
   module load cuda/7.5-fasrc01
OpenACC

On Odyssey the PGI OpenACC compiler suite is installed in /n/seasfs03/IACS/cs205/pgi. To make the compilers (pgcc, pgc++, pgf90, etc.) available in your path, add the following lines to your .bashrc file (assumes you are using bash, which is the default shell):

```
export PGI=/n/seasfs03/IACS/cs205/pgi
export PATH=$PGI/linux86-64/17.10/bin:$PATH
export MANPATH=$MANPATH:$PGI/linux86-64/17.10/man
export LM_LICENSE_FILE=$LM_LICENSE_FILE:$PGI/license.dat
```

Once you add these to your ~/.bashrc, to make these take effect, you can do, in a terminal:

```
source ~/.bashrc
```

or

```
~/.bashrc
```

or you can log out and log back in.

Using OpenACC

You need to first compile your code (say code_acc.c or code_acc.f90) containing OpenACC (see below for example programs).

Note that pgcc and pgf90 should be available in your path for this to succeed (see above for instructions).

For c program:

```
pgcc -Minfo=accel code_acc.c
```

For fortran program:

```
pgf90 -Minfo=accel code_acc.f90
```

will create an executable with name a.out. The option -Minfo=accel will display useful information on parallelization.

Slurm Script for running the job on odyssey:

```
#!/bin/bash
#SBATCH -N 1  #Number of nodes
#SBATCH -p holyseasgpu  #Partition to submit to
#SBATCH --ntasks-per-node 2
#SBATCH --gres=gpu:1
#SBATCH -t 15  #Runtime in minutes
./a.out
```

Links on OpenACC (with tutorials and sample OpenACC programs)

1) OpenACC example programs

On Odyssey, you can find the OpenACC example programs in:
Introduction to OpenACC (with sample code including Laplace) is in:

https://www.psc.edu/images/xsedetraining/OpenACCDec2016/OpenACC_Introduction_To_OpenACC.PDF

Introductory OpenACC tutorial (free, but requires an account):

https://nvidia.qwiklab.com/quests/3?locale=en

PyCuda

Using PyCuda on Odyssey

The modules that need to be loaded for using pycuda on odyssey are as under (after sourcing new-modules.sh if you have not done that):

module load Anaconda/1.9.2-fasrc01
module load cuda/7.5-fasrc01
module load pycuda/2015.1.3-fasrc01

Pycuda examples come with the pycuda distribution. You can clone the pycuda repository as:

git clone --recursive http://git.tiker.net/trees/pycuda.git

The examples are in the directory:

pycuda/examples/

Using the example "demo_elementwise.py" (demo_elementwise.py), a sample slurm script would be (pycuda_submit_wiki.sh)

-------------------------------
#!/bin/bash
#SBATCH -p holyseasgpu
#SBATCH -n 4
#SBATCH --gres=gpu:1
#SBATCH --mem-per-cpu=4000
# Load required modules
source new-modules.sh
module load Anaconda/1.9.2-fasrc01
module load cuda/7.5-fasrc01
module load pycuda/2015.1.3-fasrc01
module list
# Run program
python demo_elementwise.py
-------------------------------

(The example "dump_properties.py" (in pycuda/examples) will list the properties of cuda node on which slurm ran)

PyCuda links
PyOpenCL

Using PyOpenCL on Odyssey

The module that needs to be loaded for using PyOpenCL on odyssey is "pyopencl". Thus, one needs to do:

source new-modules.sh

module load pyopencl

before PyOpenCL can be used.

PyOpenCL examples come with the PyOpenCL distribution. You can clone the PyOpenCL repository as:

```
git clone --recursive http://git.tiker.net/trees/pyopencl.git
```

The examples are in the directory:

```
pyopencl/examples/
```

Using the example "demo_elementwise.py", a sample slurm script would be:

```
#!/bin/bash

#SBATCH -J elementwise_pyopencl
#SBATCH -o elementwise.out
#SBATCH -e elementwise.err
#SBATCH -p holyseasgpu
#SBATCH -n 2
#SBATCH --gres=gpu:1
#SBATCH --mem-per-cpu=500

# Load required modules
export PYOPENCL_CTX=""
source new-modules.sh
module load pyopencl

# Run program
python demo_elementwise.py
```
3) https://www.khronos.org/opencl/