EPL372
Hands on training session

Thekla Loizou

The Cyprus Institute

Overview

- Cy-Tera
- Euclid
- How to access Euclid (ssh)
- Software Environment (Modules)
- Hands on exercises

Cy-Tera

- Hybrid CPU/GPU Linux Cluster
- Computational Power
  - 98 x 2 x Westmere 6-core compute nodes
  - 18 x 2 x Westmere 6-core + 2 x NVIDIA M2070 GPU nodes
- Theoretical Peak Performance (TPP) = 30.5Tflops
  - Each compute node = 128GFlops
  - Each GPU node = 1 Tflop
- 48 GB memory per node
- 40Gbps QDR Infiniband
- Storage: 360TB raw disk

Euclid

- Training Cluster
- Hybrid CPU/GPU Linux Cluster
- Computational Power
  - 6 eight-core compute nodes + 2 NVIDIA Tesla T10 processors
- Theoretical Peak Performance (TPP) = 0.5 Tflop/s
- 16 GB memory per node
- Infiniband Network

How to access Euclid

- To access the system you must have access to your private key:
  - If the key is stored in your .ssh folder in your home directory:

```
ssh username@euclid.cyi.ac.cy
```

  - If the key is stored in another directory or in a usb:

```
ssh –i /key_path/id_rsa username@euclid.cyi.ac.cy
```

  - Your key should only be readable and writable by you. If not, please go to the directory where your key is stored and change its permissions accordingly:

```
chmod 600 id_rsa
```

Environment Setup with Modules

- The software environment used on Cyl systems can be managed via Modules
- Modules facilitate the task of updating applications and provide a user-controllable mechanism for accessing software revisions and controlling combination of versions
- Useful module commands
  - **`module avail`** : list all available modules
  - **`module load X`** : load module X
  - **`module unload X`** : unload module X
  - **`module list`** : list currently loaded modules
  - **`module whatis X`** : display information for module X
  - **`module purge`** : unload all loaded modules

Modules on Euclid

```
------------------------------------------------------------ /fhgfs/euclid/buildsets/eb141014/modules/all ------------------------------------------------------------
   ATLAS/3.10.1-gompi-1.5.12-LAPACK-3.4.2                    OTF2/1.4-ictce-5.3.0                                (D)    hello/0.1-ictce-5.3.0                              (D)
   Autoconf/2.69-GCC-4.8.2                                   OpenBLAS/0.2.6-gompi-1.3.12-LAPACK-3.4.2                  hwloc/1.6.2-GCC-4.6.4
   Autoconf/2.69-gcccuda-2.6.10                      (D)     OpenBLAS/0.2.6-gompi-1.4.10-LAPACK-3.4.2                  hwloc/1.6.2-GCC-4.7.2
   Automake/1.14-GCC-4.8.2                                   OpenBLAS/0.2.8-gompi-1.5.12-LAPACK-3.4.2                  hwloc/1.7.2-GCC-4.8.2
   Automake/1.14-gcccuda-2.6.10                      (D)     OpenBLAS/0.2.8-gompi-1.6.10-LAPACK-3.4.2                  hwloc/1.8-gcccuda-2.6.10
   Bison/2.5-GCC-4.6.3                                       OpenBLAS/0.2.8-gompic-2.6.10-LAPACK-3.4.2         (D)     hwloc/1.9-GCC-4.8.3
   Bison/2.5-goolf-1.4.10                                    OpenMPI/1.6.4-GCC-4.6.4                                   hwloc/1.10.0-GCC-4.9.2                             (D)
   Bison/2.7-GCC-4.7.3                                       OpenMPI/1.6.4-GCC-4.7.2                                   icc/2011.13.367
   Bison/2.7-goolf-1.4.10                                    OpenMPI/1.6.5-GCC-4.8.1                                   icc/2013.3.163                                     (D)
   Bison/2.7-goolf-1.6.10                                    OpenMPI/1.7.3-GCC-4.8.2                                   iccifort/2011.13.367
   Bison/2.7-ictce-5.3.0                             (D)     OpenMPI/1.7.3-gcccuda-2.6.10                              iccifort/2013.3.163                                (D)
   CMake/2.8.4-goolf-1.4.10                                  OpenMPI/1.8.1-GCC-4.8.3                                   ictce/4.1.13
   CMake/2.8.12-goolf-1.4.10                                 OpenMPI/1.8.4-GCC-4.9.2                           (D)     ictce/5.3.0                                        (D)
   CMake/2.8.12-goolfc-2.6.10                        (D)     PAPI/5.2.0-ictce-5.3.0                                    ifort/2011.13.367
   CUDA/5.0.35-1                                             PAPI/5.3.2-gompi-1.6.10                                   ifort/2013.3.163                                   (D)
   CUDA/5.5.22-GCC-4.8.2                                     PAPI/5.3.2-ictce-5.3.0                            (D)     iimpi/4.1.13
   CUDA/5.5.22                                       (D)     PDT/3.19-gompi-1.6.10                                     iimpi/5.3.0                                        (D)
   CosmoloPy/0.1.104-goolf-1.4.10-Python-2.7.3               PDT/3.19-ictce-5.3.0                              (D)     imkl/10.3.12.361-iimpi-4.1.13
   Cube/4.2-goolf-1.4.10                                     PP/1.6.4-goolf-1.4.10-Python-2.7.3                        imkl/11.0.3.163-iimpi-5.3.0
   Cube/4.2.3-gompi-1.6.10                                   PP/1.6.4-ictce-5.3.0-Python-2.7.3                 (D)     imkl/11.0.3.163                                    (D)
   Cube/4.2.3-ictce-5.3.0                            (D)     Python/2.5.6-gompi-1.6.10-bare                            impi/4.1.0.027-iccifort-2011.13.367
   Doxygen/1.8.1.1-goolf-1.4.10                              Python/2.5.6-goolf-1.4.10-bare                            impi/4.1.0.030-iccifort-2013.3.163
   Doxygen/1.8.3.1-goolf-1.4.10                              Python/2.7.3-goolf-1.4.10                         (D)     impi/4.1.0.030                                     (D)
   Doxygen/1.8.3.1-ictce-5.3.0                       (D)     Python/2.7.3-ictce-4.1.13                                 inputproto/2.3-ictce-5.3.0
   EasyBuild/1.10.0                                          Python/2.7.3-ictce-5.3.0                                  ipp/7.0.5.233
   EasyBuild/1.15.2                                  (D)     Python/3.2.3-goolf-1.6.10                                 itbb/4.2.5.176
   FFTW/3.3.3-gmvapich2-1.7.12                               Python/3.3.2-goolf-1.4.10                                 kbproto/1.0.6-ictce-5.3.0
   FFTW/3.3.3-gompi-1.3.12                                   Qt/4.8.4-goolf-1.4.10                                     libX11/1.6.1-ictce-5.3.0
   FFTW/3.3.3-gompi-1.4.10                                   Qt/4.8.5-gompi-1.6.10                                     libXau/1.0.8-ictce-5.3.0
   FFTW/3.3.3-gompi-1.6.10                                   Qt/4.8.5-ictce-5.3.0                              (D)     libffi/3.0.13-gompi-1.6.10
   FFTW/3.3.3-gompic-2.6.10                          (D)     SIONlib/1.5.2-gompi-1.6.10                                libffi/3.0.13-goolf-1.4.10
   GCC/4.6.3                                                 SIONlib/1.5.2-gompi-2015a                                 libffi/3.0.13-ictce-5.3.0                          (D)
   GCC/4.6.4                                                 ScaLAPACK/2.0.2-gompi-1.3.12-OpenBLAS-0.2.6-LAPACK-3.4.2  libpng/1.5.13-goolf-1.4.10
   GCC/4.7.2                                                 ScaLAPACK/2.0.2-gompi-1.4.10-OpenBLAS-0.2.6-LAPACK-3.4.2  libpng/1.5.13-ictce-5.3.0
   GCC/4.7.3                                                 ScaLAPACK/2.0.2-gompi-1.6.10-OpenBLAS-0.2.8-LAPACK-3.4.2  libpng/1.6.6-goolf-1.4.10                          (D)
   GCC/4.8.1                                                 ScaLAPACK/2.0.2-gompic-2.6.10-OpenBLAS-0.2.8-LAPACK-3.4.2 (D)  libreadline/6.2-gompi-1.6.10
   GCC/4.8.2                                                 Scalasca/2.0-goolf-1.4.10                                 libreadline/6.2-goolf-1.4.10
   GCC/4.8.3                                                 Scalasca/2.1-ictce-5.3.0                          (D)     libreadline/6.2-goolf-1.6.10
   GCC/4.9.2                                         (D)     Score-P/1.3-ictce-5.3.0                           (D)     libreadline/6.2-ictce-4.1.13
   GDL/0.9.3-goolf-1.4.10                                    Szip/2.1-goolf-1.4.10                                     libreadline/6.2-ictce-5.3.0                        (D)
   GLib/2.34.3-gompi-1.6.10                                  Szip/2.1-ictce-5.3.0                              (D)     libxcb/1.8-ictce-5.3.0-Python-2.7.3
   GLib/2.34.3-goolf-1.4.10                                  Tcl/8.5.12                                                make/3.82-goolf-1.4.10
   GLib/2.34.3-ictce-5.3.0                           (D)     Valgrind/3.8.1-goolf-1.4.10                               matplotlib/1.2.1-goolf-1.4.10-Python-2.7.3         (D)
   GROMACS/4.6.1-goolf-1.4.10-hybrid                         WRF/3.4-goolf-1.4.10-dmpar                                matplotlib/1.2.1-ictce-5.3.0-Python-2.7.3
   GROMACS/4.6.5-goolf-1.4.10-hybrid                         WRF/3.4-ictce-5.3.0-dmpar                         (D)     matplotlib/1.3.1-goolf-1.4.10-Python-3.3.2
   GROMACS/4.6.5-goolf-1.4.10-mt                     (D)     arpack-ng/3.1.3-ictce-5.3.0                               mpi4py/1.3-goolf-1.4.10-Python-2.7.3
   GSL/1.16-goolf-1.4.10                                     astropy/1.0.6-goolf-1.4.10-Python-2.7.3           (D)     ncurses/5.9-gompi-1.6.10
   HDF5/1.8.9-goolf-1.4.10                                   astropy/1.0.6-goolf-1.4.10-Python-3.3.2                   ncurses/5.9-goolf-1.4.10
   HDF5/1.8.10-patch1-goolf-1.4.10                           binutils/2.24                                             ncurses/5.9-goolf-1.6.10
   HDF5/1.8.10-ictce-5.3.0-gpfs                      (D)     bzip2/1.0.6-gompi-1.6.10                                  ncurses/5.9-goolfc-2.6.10
   HPL/2.0-goolf-1.4.10                                      bzip2/1.0.6-goolf-1.4.10                                  ncurses/5.9-ictce-4.1.13
   HPL/2.0-ictce-5.3.0                               (D)     bzip2/1.0.6-goolf-1.6.10                                  ncurses/5.9-ictce-5.3.0                            (D)
   IOR/2.10.3-goolf-1.4.10-mpiio                             bzip2/1.0.6-ictce-4.1.13                                  netCDF/4.2.1.1-goolf-1.4.10
   JasPer/1.900.1-goolf-1.4.10                               bzip2/1.0.6-ictce-5.3.0                           (D)     netCDF/4.2.1.1-ictce-5.3.0                         (D)
--More--
```

Hands on exercises

- Copy the hands on exercises directory into your home directory:
  - If you are not in your home directory first type “cd”

```
cp -r /opt/exercises .
```

- Go into the exercises directory:

```
cd exercises
```

Steps to run a code

1. Load the modules needed to compile the code
2. Compile the code
3. Create a job script
    - The job script will be submitted to the queue
    - Job script asks for resources to run the compiled code
    - Through the job script the code will run on the compute nodes
4. Submit job script

Exercise 1- MPI Hello World

```
#include <stdio.h>
#include <mpi.h>
int main(int argc, char ** argv) {
int size,rank;
int length;
char name[80];

MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
MPI_Comm_size(MPI_COMM_WORLD,&size);
MPI_Get_processor_name(name,&length);

printf("Hello MPI World! Process %d out of %d on %s\n",rank,size,name);
MPI_Finalize();
return 0;
}
```

Exercise 1 - Compile the code

- Load the goolf module (g - GCC compiler, o - OpenMPI, o - OpenBLAS, l - ScaLAPACK, f - FFTW)

```
module load goolf
```

- Compile the code

```
mpicc hello.c -o hello
```

Exercise 1 - Create job script

```
#!/bin/bash

#SBATCH --job-name=hello-world
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=8
#SBATCH --time=00:01:00
#SBATCH --error=hello.out
#SBATCH --output=hello.out

module load goolf/1.6.10

mpirun -np 16 ./hello
```

Exercise 1 - Submit job to queue

- Submit the job to the queue

```
sbatch hello.sub
```

- Check the queue status

```
squeue
```

- Check the contents of the output file

```
cat hello.out
```

Exercise 2 - CUDA devices accessible by each process

- Load the goolf (g - GCC compiler, o - OpenMPI, o - OpenBLAS, l - ScaLAPACK, f - FFTW) and CUDA modules:

```
module load goolf

module load CUDA
```

- Compile the code

```
nvcc -lmpi mpi-cuda.cu -o mpi-cuda
```

Exercise 2 - Create job script

```
#!/bin/bash

#SBATCH --job-name=mpi-cuda
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=8
#SBATCH --time=00:01:00
#SBATCH --gres=gpu:2
#SBATCH --error=mpi-cuda.out
#SBATCH --output=mpi-cuda.out

module load CUDA/5.5.22
module load goolf/1.6.10

mpirun -np 8 ./mpi-cuda
```

Exercise 2 - Submit job to queue

- Submit the job to the queue

```
sbatch mpi-cuda.sub
```

- Check the queue status

```
squeue
```

- Check the contents of the output file

```
cat mpi-cuda.out
```

Thank you!

Questions?