# Cray CX1 at IUCAA

An Overview

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Sept 07, 2011

#### CRAY CX1: Front and back view





#### CRAY CX1: motherboard



#### CRAY CX1: Control panel







#### Overview

- Cray CX1 is a desktop/desk-side supercomputer with 1 head node, 1 GPU node and 4 compute nodes.
- ► Each node has two 2.67 Ghz Intel Xeon(5650) processors, with every processor having six cores.
- In total there are 72 cores on the systems. Since there are twelve cores on every node, one can use twelve OpenMP hardware threads.
- Every node has 24 GB RAM and in total the system has 144 GB RAM.
- At present there is around 5 TB disk space available for users on three different partitions, named /home, /data1/ and /data2.
- ► Theoretical computing power of the system on CPU is 768.96 GF and on GPU is 515 GF (with 3GB Memory).

### Compilers

- Names of the nodes are as hpccmb (head node), compute-00-00 (GPU node) and compute-00-01, compute-00-02 and , compute-00-04.
- ► There are many software, packages and libraries already installed in the system and more (open source) can be installed. At present the system has the following compilers:
  - 1. gcc version 4.1.2 ( **gfortran** and **gcc**).
  - Compilers supplied with the platform system ( mpicc, mpiCC, mpif77, mpif90 etc.,) are installed in "/opt/platform\_mpi/".
  - Open MPI compilers ( mpic++ ,mpicc, mpiCC, mpicxx, mpiexec, mpif77 etc.,) installed in "/data1/software/openmpi".
  - Intel compilers ( icc and ifort) are installed in "/opt/intel/".
     In this area Intel Mathematical Kernel Library (MKL) and Intel Threading Building Blocks (ITBB) are also installed.

### **Packages**

- ▶ Platform LSF is successfully running on the system and by default all MPI jobs will be assigned in a "batch queue" mode.
- In general, users are not needed to specify the nodes to which they want to assign the job, however, it may be useful in some cases.
- The system already has many scientific packages/libraries pre-installed or have been installed, some of them are as follows:
  - blacs, linpack, scalapack and hdf5 supplied with the system are installed in "/opt".
  - 2. **gnuplot, gv, acoread** etc., are installed.
  - 3. A good number of packages including **fftw2**, **fftw3**, **pgplot**, **cfitsio**, **lapack** are installed in "/data1/software".
  - 4. Some of the packages related to CMBR work ( cmbfast, camb, cosmomc, healpix etc.,) are already been installed in "/data1/soft\_cmbr/" and more will be installed.

#### Running the Jobs

▶ Job on the system can be submitted using two different modes. In the first case job can be submitted using a platform GUI supplied with the system which can be accessed at the following URL from the IUCAA network.

```
http://192.168.11.243:8080/platform/,
```

Jobs can be submitted from the terminal also and a typical MPI submission script may look like:

```
mpirun -np 32 -hostlist "compute-00-00,compute-00-01,compute-00-02,compute-00-04" \ ./cosmomc params.ini
```

apart from this the direct submission also works:

```
mpirun -np 4 ./a.out
```

I think one of the most useful ways to submit a MPI job, particularly when it uses OpenMP also is by using the *appfile*. Create an appfile with the following content:

```
cat appfile
-h compute-00-01 -np 2 ./cosmomc params.ini
-h compute-00-02 -np 2 ./cosmomc params.ini
-h compute-00-03 -np 2 ./cosmomc params.ini
-h compute-00-04 -np 2 ./cosmomc params.ini
```

Once appfile is created it can be run using the following command.

```
mpirun -f appfile
```

## **GPU** Computing

► The system has one Nvidia Tesla C2050 GPU which is hosted on the node **compute-00-00**. Detail status of the GPU can be printed on the standard output using the the **nvidia-smi** command one of its example is as follows:

nvidia-smi -q

This will print a lot of useful information about the GPU. You can use "-help" option also to find all the option available for **nvidia-smi**.

- Compute Unified Device Architecture (CUDA) library as well as the compiler **nvcc** is installed in the are "/usr/local/cuda". In order to run a cuda program, follow the following three steps:
  - Write a source/program file with suffix ".cu" following the cuda syntax.
  - Compile the program with nvcc: nvcc prog.cu
  - ▶ Run the executable: ./a.out

#### Specs of the GPU

```
--- General Information for device 0 ---
Name: Tesla C2050
Compute capability: 2.0
Clock rate: 1147000
Device copy overlap: Enabled
Kernel execition timeout : Disabled
--- Memory Information for device 0 ---
Total global mem: 2817982464
Total constant Mem: 65536
Max mem pitch: 2147483647
Texture Alignment: 512
--- MP Information for device 0 ---
Multiprocessor count: 14
Shared mem per mp: 49152
Registers per mp: 32768
Threads in warp: 32
Max threads per block: 1024
Max thread dimensions: (1024, 1024, 64)
Max grid dimensions: (65535, 65535, 65535)
```

Thank You!