Minutes of CCCC Meeting held on January 20, 2011

Members present: Madhav Ranganathan, Raj Pala, A.K. Saha, P.M. Mohite, Dheeraj Sanghi, Vimal Kumar, Sudib Mishra, Abhijit Chatterjee, P.A. Apte, R. Sankararamakrishnan, S. Mittal, K.S. Singh, Brajesh Pande, Gopesh Tiwari, Aftab Alam, A. Chandra

Head CC welcomed all the members of CCCC and special Invitees. Subsequent proceedings of the Meeting are given below.

1. The minutes of the previous CCCC meeting held on December 16, 2010, were confirmed.

2. Head CC made the following announcements:

    (i) The process of purchase of the new Internet Gateway Security Solution (Cisco), which was discussed in the previous CCCC meeting, is underway and the purchase order is expected to be released in a week.

    (ii) The new UPS System (4 x 300 KVA) is now up and working fine.

    (iii) IWD would be starting renovation (civil) work in the ground floor of CC very soon. All CC Engineers (except Saikat Hira) would move to the second floor of CC for the duration of the IWD work. The Windows PC Lab in the ground floor would also be shut down permanently as this space would become part of the Data Centre that would be constructed in the ground floor.

    (iv) The smaller Linux Lab in the second floor of CC (Room 217) would be converted to HPC visualization, data analysis cum Visitors' Lab. It was noted that ESC101 Lab classes are now taking place in the New Core labs, hence three PC labs (L1, L2 and L3 with L2 operating in both Windows and Linux modes) should be sufficient to meet other PC Lab related requirements of CC users.

3. Subsequently, the main agenda item of HPC usage policy was taken up. Head CC informed the members that the main (new) HPC facility consisting of a Linux cluster of 372 nodes with 100 TB disk and 40Gbps Infiniband Network is expected to be released to users in about two weeks. In addition to this, the members were also informed of the procurement of four GPU servers and six high-end Workstations for computing and visualization purposes, respectively. Regarding the usage of the main HPC facility, i.e. the 372-node cluster, Head CC made a presentation on the cluster with brief outlines of the hardware and software that are available in the cluster (or would be available shortly) and a proposed usage policy with a scheme of batch queues and suggestions on handling of day-to-day issues (copy of the presentation is included in the Appendix). The main points of the proposed usage policy include:

Job Queues

Queue	Nodes	Min nodes (cores)	Max nodes (cores)	Wall time
Large	184	16 (128)	32 (256)	3 days
Medium	92	4 (32)	12 (96)	4 days
Small	46	1 (8)	4 (32)	5 days
Seq	32*	1 (1)	1 (1)	6 days

(* max 8 jobs per user, max 32 users, Seq means sequential)

Interactive (visualization, Testing)	12	Free flow (CPU time: 2 hrs; Wall time: 2 days)	

Number of jobs a user can run

A user will be allowed to run one job and keep another job waiting in each queue.

Users of the new HPC facility

- Users of HP and SUN clusters will be given accounts in the new HPC cluster
- New faculty HPC users will be given accounts on request. For students, the request for account in the new HPC cluster will have to routed through thesis supervisor(s). Specific recommendation of thesis supervisor(s) will be required.

Old Clusters

(Old) HP cluster will be turned on and will be made available for use for courses. SUN Cluster would be turned on only when the new Data Centre has come up.

Handing of day-to-day issues

- Basic documentation for users will be provided online
- Application package related problems should be posted on HPC users forum (hpc@lists.iitk.ac.in). For each major software, a faculty adviser should be identified. He would look at the problem for that particular software and provide necessary answer to the user through hpc@lists.iitk.ac.in. It is expected that a pool of faculty and students would be created over time who would handle this job of addressing application package related problems. CC solicits faculty volunteers for this purpose.
- All system related issues including job scheduler and announced compilers should be reported to brajesh@iitk.ac.in.

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A long discussion took place on each of the items mentioned above. The members generally agreed with the proposed batch queues. However, concerns regarding too many non-HPC users getting accounts and running jobs in the Seq queue which otherwise could be run in normal

servers were expressed. Members opined that CC could look into the possibility of purchase of some additional servers with large memory for users of serial computing and once that happens, the Seq queue should be taken off from the HPC cluster. Till that time, members approved that the batch queues as given above would be put in operation. The System Administrator of the new HPC cluster informed that the interactive queue may in practice be operating with one less node in the initial period because of system administrative reasons.

Members approved the proposed number of jobs for a user that would be permitted, i.e. one job running and another allowed to be waiting in a given queue. Regarding the allowed users of the HPC cluster, members approved the policy outlined above. However, it was stressed that this facility is primarily for parallel computing and, hence, access to users of serial computing should be given only in cases where the extent of required serial computing is truly demanding. Thesis supervisors of student users should be requested to keep this aspect in mind before recommending his/her students for accounts in the new cluster.   The proposed use of the old HP cluster for courses was then discussed. While the members welcomed the idea, it was suggested that this facility should also be made available for research-related usage. Hence, it was decided that HP cluster would be turned on and released to all its users as early as possible. The handing of day-to-day issues of the HPC facility was then discussed and the proposed policy was approved. Head CC stressed the need for having a set of faculty and student volunteers and hoped that some of the HPC users would come forward to offer their help in addressing application package related issues voluntarily. The Meeting ended with thanks to the Chair.
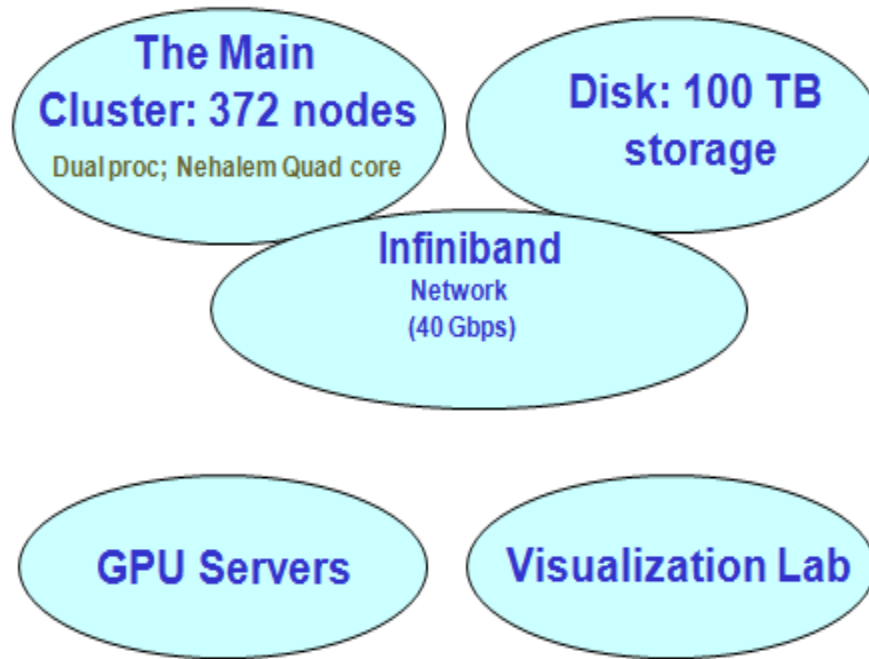
Head, Computer Centre
IIT Kanpur

Annexure 1

Presentation made by Head, CC, at the CCCC

Meeting on January 20, 2011

New HPC Facility at CC

The New HPC Setup

The Main Cluster: 372 nodes

Dual proc; Nehalem Quad core

Disk: 100 TB storage

Infiniband
Network
(40 Gbps)

GPU Servers

Visualization Lab

Software

Compilers and job scheduler

- **Intel suite of compilers (Fortran, C/C++) and Math libraries**
- **Intel MPI**
- **MPICH2: gcc, gfortran, icc ifort (32, 64)**
- **MVAPICH2: various flavors**
- **PBS Pro (job scheduler)**
- **PGI Suite of compilers**
- **PBS Portal**

Application packages:

Following packages have been run during testing phase

CPMD (Earlier benchmarks essentially reproduced)
GROMOS
CHARMM
CFD and other parallel codes from various groups

Software ordered/procured (parallel versions):

Accelrys. Ansys, Fluent, Turbomole, Gaussian, Matlab, NAG, Tecplot

Several open source packages

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