

I.1: Scientific computing and software development at RRCAT

A) Commissioning of InfiniBand based High Speed Interconnect for Centralized Computing Server Setup:

Centralized computing server setup comprises of servers with different Linux flavour like – RedHat Linux version 7.2/ 9, Red Hat Enterprise Linux version 3/ 4/ 5 on different hardware architectures like – Compaq alpha, Intel Itanium, Intel Xeon, IBM Power 5 etc. This setup is used by nearly 125 scientists and engineers for running their scientific and engineering applications. Centralized access of MATLAB, ANSYS, MATHEMATICA and ELMERFEM software packages has also been provided through this setup. All these packages provide features like simulation and graphical presentation. 40 Gbps InfiniBand interconnect has been commissioned to provide improved performance and enhanced graphical support for scientific & engineering applications. This high speed interconnect based setup comprises of 4X QDR InfiniBand switch and InfiniBand HCA (Host Channel Adapter) cards for individual servers.

This InfiniBand interconnect is working along with Gigabit Ethernet switch and it supports earlier applications also.

B) Commissioning of Itanium-2 based Computing Server for centralized access of Ansys version 14:

Computing server named as **Ganak-2 (गणक-2)** comprising of two, dual core 1.6 GHz Itanium-2 based 64-bit processors with 18 MB L3 cache and 64 GB RAM has been commissioned for centralized access of Ansys software version 14. This server is configured with InfiniBand interconnect. Red Hat Enterprise Linux Server release 5.7 is used as operating system for this server. Intel C & FORTRAN compilers version 11.1 and Math Kernel Library version 11 are configured for advanced computing and engineering applications.

Ansys version 14 has been installed and users can run their applications of Ansys from their desktops (Windows/ Linux).

C) 3D Visualization of New Data Centre Hall:

A software module has been devised for 3D visualization of Data Centre Hall (DCH) located at IT Extension building for helping in space and resource management. This will help to find suitable place for installing any device in data centre using Walkthrough of DCH in 3D thus resulting in proper space utilization.

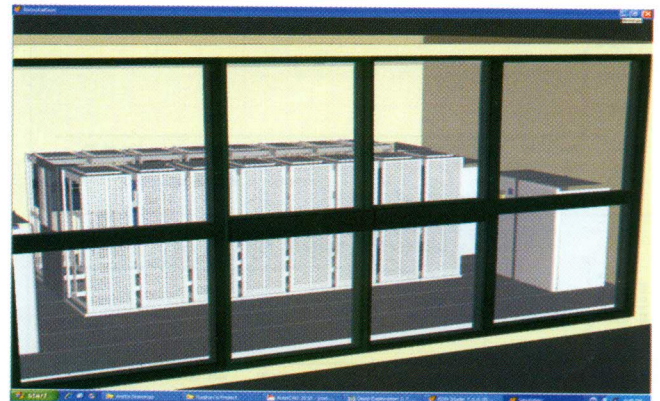


Figure I.1.1: 3D Visualization of Data Centre Hall located at IT Extension building, RRCAT.

The development of this system included importing 3D objects, usually originating from AutoCAD. Behavior is associated with the models through intuitive graphical programming interface and scripting available in EON software. Visualization in 3D and walkthrough of Data Centre virtually is possible with the help of Stereo Projection System, Front Projection Screen, Stereo Emitter and Stereo Eyewear. This software is helpful in future planning also, for placement of devices in an optimum way.

D) Web based monitoring tools for LDAP based Computing Server Setup:

Web based monitoring tool has been developed and configured for LDAP based computing server setup to monitor the CPU load, total running processes, memory & swap usage and network traffic etc. Users' details like login details and disk usage on respective server can also be reported through this software.

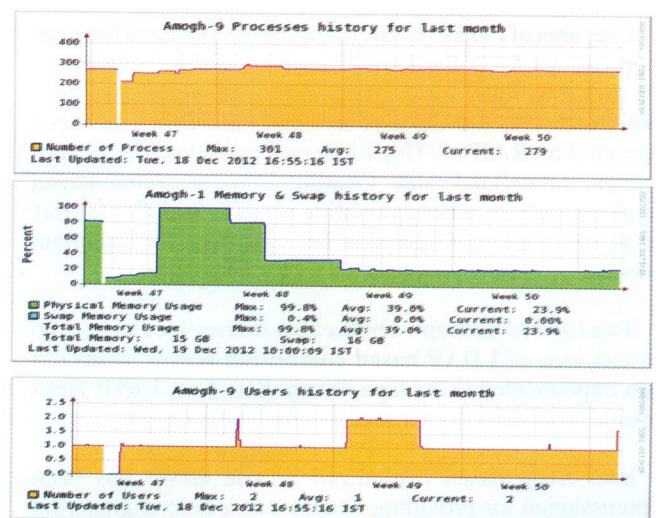


Figure I.1.2: Processes, memory usage and number of users logged on computing servers.

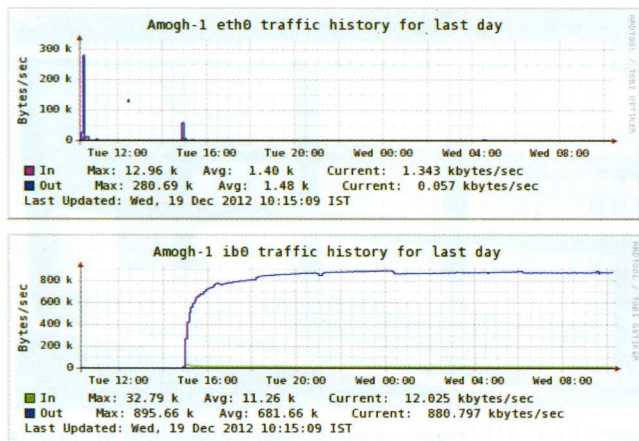


Figure I.1.3: Traffic profile of Amogh-1 server for Ethernet and InfiniBand switch based setups.

This software has been developed using open source RRDtool (Round Robin Database tool), HTML and PHP programming language. RRDtool handles time-series data like network bandwidth, temperature, CPU load etc. The data is stored in a round-robin database (circular buffer). It also includes tools to extract RRD data in a graphical format. The advantage of using RRDtool is that the image contains dynamically updated current and average data.

Deployment of this monitoring tool has eased the task of system administration and has also enhanced resource utilization.

E) Augmentation of Centralized Computing Server Setup:

User area of LDAP based computing server setup has been upgraded to 1.5 TB. Earlier we had single file server with 800 GB user area. Intel Xeon based Linux file server has been configured with 700 GB user area and redundancy has been supported by RAID-6. This file server provides file services through InfiniBand and Gigabit Ethernet interconnect simultaneously to other computing servers. Standby for this file server is also configured in fail safe mode for important user data.

Two layered backup – Differential & Incremental backup for user area of **LDAP based computing server setup** has been implemented using tape library. Set of six 1.6TB tapes are used for both Differential & Incremental backups.

Intel Xeon based centralized license server has been commissioned for providing license services to engineering and scientific application software packages.

F) Porting of user programs:

As per requirement of users, following parallel and sequential application packages are successfully ported on clusters and computing servers:

Following three software packages have been ported and used by Indus Synchrotrons Utilization Division:

Quantum ESPRESSO on HPC cluster

Quantum ESPRESSO (opEn Source Package for Research in Electronic Structure, Simulation, and Optimization) has been successfully ported on HPC cluster Kshitij-2. Quantum ESPRESSO is an integrated suite of Open-Source computer codes for electronic-structure calculations and material modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudo potentials.

Quantum ESPRESSO version 5.0 has been ported using Intel FORTRAN & C compiler, MKL Library and OPENMPI version 1.4.2. It was also configured through resource manager - TORQUE & scheduler – MAUI of HPC cluster, Kshitij-2.

Yambo

Parallel application **Yambo** (A computer program based on Main-body perturbation theory for calculation of electronic and optical properties in Solid State and Molecular Physics) has been successfully ported on HPC cluster Kshitij-2 using FORTRAN & C compiler, MKL Library and OPENMPI version 1.4.2.

CASTEP and Material Studio

CASTEP (a state-of-the-art quantum mechanics-based program designed specifically for solid-state materials science) has been successfully configured on HPC cluster Kshitij-2. This parallel application package bundled with Intel MPI Library has been configured using Intel Fortran compiler and resource manager - TORQUE & scheduler – MAUI. Its windows portal **Material Studio version 6.0** was also configured for submitting jobs to HPC cluster Kshitij-2.

Dimad

Dimad (this program studies particle behaviour in beam lines and circular machines) has been successfully ported on Intel based Linux server with **Extended Standard Input Format (XSIF)** library and Intel FORTRAN compiler. XSIF was configured and then DIMAD was ported using XSIF library. This application is used by Indus Operations and Accelerator Physics – Design Division.

Radia module for **Mathmatica** version 7.0 has been configured on Intel based Linux server for Accelerator Magnet Technology Division.

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