I.1 Scientific Computing and Software Development at RRCAT

A) Augmentation of Centralized Computing Server Setup:

Computing servers named as **Amogh-7** (अमोघ-7), **Amogh-8** (अमोघ-8), **Amogh-9** (अमोघ-9) and **Amogh-10** (अमोघ-10) have been commissioned for scientific computing and engineering applications. Each server has two Intel Xeon 3.6 GHz Quad core processors and 32 GB memory. Operating system of Amogh-7, Amogh-8 and Amogh-9 is Red Hat Enterprise Linux Server release 5.7 (64Bit X86_64). Scientific Linux release 6.1 (64Bit X86_64) is used as operating system of Amogh-10. Intel C & FORTRAN compilers version 11 & Math Kernel Library version 11 are configured on Amogh-8 and Amogh-9 servers. Intel C & FORTRAN compilers version 12 & Math Kernel Library version 12 are configured on Amogh-7 & Amogh-10 servers for advanced applications.

ATLAS (Automatically Tuned Linear Algebra Software) is also installed on these servers for GNU C & FORTRAN compilers. GNU Multiple Precision Arithmetic Library (gmp version 5.0.2), Multiple Precision Complex Library (mpc version 0.9), Multiple Precision Floating-Point Reliable Library (mpfr version 3.0.1) and GNU Compiler Collection (GCC version 4.5.3) are also configured to support latest GUI based scientific & engineering applications.

B) Commissioning of High Resolution Multi-screen Tile Display:

High resolution multi-screen tile display has been commissioned by tiling four LCD displays driven by Windows based graphics rendering workstation. This 4-tile (2x2) LCD display system has been designed to provide a display resolution of 3840x2160 (8.2 million) pixels. Each tile is 46″ GoodView PD46N4 display with resolution of 1920x1080 pixels. Windows 7 based graphics workstation with two Intel Xeon X5680 hex core 3.33 GHz processors, 48 GB RAM and two NVIDIA Quadro NVS 300 multi display graphics cards are used to render high resolution display.

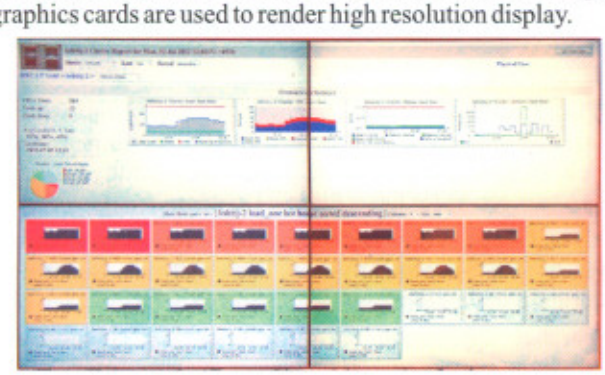

Figure I.1.1: Full view of load details of Kshitij-2 HPCC on 2x2 Tile Display

This multi-screen tile display is commissioned to visualize large datasets and images which are too large to fit in a single display without compression or simplifications.

C) Performance comparison of MPI on HPCC using Infiniband & Gigabit Ethernet Interconnect:

Analytical tests were carried out on HPCC of multi-core nodes, based on parallel execution using MPI with two different types of interconnects - Gigabit Ethernet & InfiniBand (20 Gbps). Intel HPL benchmarking software – MP_LINPACK and NAS (Numerical Aerodynamic Simulation) Parallel Benchmark (NPB) were used to compare performance of MPI on both Interconnects.

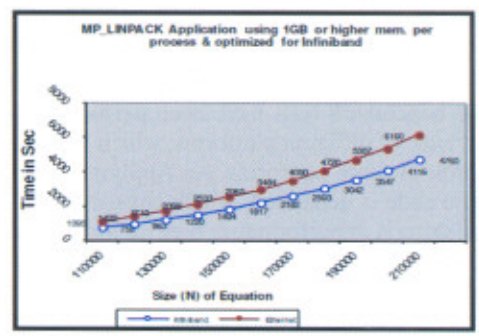

Figure I.1.2: MP_LINPACK performance chart for Infiniband & Gigabit Ethernet

For MP_LINPACK, tests were carried out for different size (N) of system equations varying from 40,000 to 2,10,000 with a step size of 10,000. To carry out these tests 128 processing cores have been used for single parallel application.

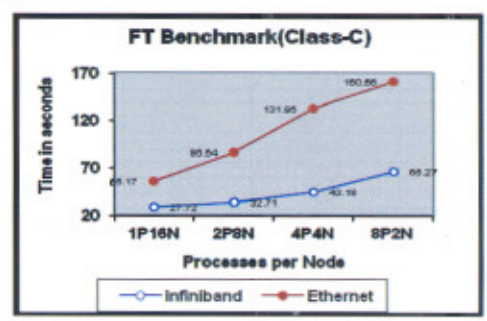

Figure I.1.3: Class C FT (NPB) benchmark for 16 processes on Infiniband & Gigabit Ethernet

For all eight benchmarks included in NPB, 16 parallel processes were used for single MPI application. The tests have been carried out with Class C size and four different cases i.e. one, two, four and eight processes per node.

The results show that MPI delivers significantly better performance on InfiniBand interconnect than Gigabit Ethernet interconnect. The performance increase depends on

communication scheme and number of processes per node used for parallel applications on HPCC with multi-core nodes.

D) Performance Evaluation of Computing Clusters for Improved QoS:

Scientific Infrastructure at RRCAT includes large number of servers, computing clusters and scientific applications to meet the computing needs of scientists. The architectural configurations vary in terms of processor speed, memory, cache, operating system, compilers, libraries etc., which in turn defines the suitability of a platform for any scientific application in use. To provide improved QoS (Quality of Service) to the users, in terms of increased performance and throughput, it is required to analyze user application code and find out its characteristics, to help in selecting suitable platform for executing particular program.

Certain benchmark tests have been performed to probe the performance of different platforms, which has resulted in categorization of these platforms. An Application Profile of the scientific code is generated, which consists of collection of technical criteria or performance metrics for that code. For improving QoS to the users, the information gathered in above steps have been used. A prototype web based module has been developed that guides the user towards selecting suitable cluster for his/ her application taking into account availability of the cluster.

The following figure shows application profile for the code DDSCAT. The software indicates various performance metrics for this code and based on the 'cost of computation' criteria, it indicates the best platform to run the application.

METRIC	Workstation	TestBED	Kshitij 2
Application Name	DDSCAT	DDSCAT	DDSCAT
Language	FORTRAN	FORTRAN	FORTRAN
MPI Percentage Time	69	66	66
Amount Of Data Transferred	28 MB	28 MB	28 MB
CPI	1.277	0.946	0.946
LLC Miss	0.069	0.004	0.004
Memory Bus Transaction	271840000	NA	NA
Instruction Starvation	0.002	0.282	0.282
Branch Mispredict	0.008	0.008	0.008
Execution Stalls	NA	0.218	0.218
Retire Stalls	NA	0.479	0.479
Total Execution Time	33 min	30 min	22 min
Cost Of Machine (in Lakhs)	0.3	13	300
Optimized Platform Today	Workstation		

Figure I.1.4: Application Profile for DDSCAT

This work was done by one of the team members as part of his M.Tech. degree under HBNI.

E) Installation of Lustre File System:

Lustre Parallel File System has been implemented on HPC cluster 'Kshitij-2' to optimize use of Gigabit Ethernet interconnects. This open-source file system used as Global File System in HPC environment has many advantages: scalibility, high performance, high availability, POSIX compliance, and security.

Metadata Server (MDS), Metadata Target (MDT), Object Storage Servers (OSS), Object Storage Target (OST), Lustre Network (LNET) & Lustre Clients are installed and configured on Kshitij-2 cluster. All computing nodes of Kshitij-2 are configured as clients of Lustre File System.

F) Porting of user programs:

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

VORPAL on HPC cluster

Parallel application **VORPAL** (Versatile Object oriented code for Relativistic Plasma Analysis with Laser) is successfully ported on HPC cluster, Kshitij-2 with visualization feature for Laser Plasma Division. VORPAL is used to simulate the physical behavior of devices and processes for many research and industrial applications and its visualization tool is used to visualize the simulation results.

Initially VORPAL version 5.0.0 was ported using OPENMPI and it was configured for use through resource manager - TORQUE & scheduler – MAUI of HPC cluster, Kshitij-2. These tools are essential to execute parallel application software in distributed computing mode. Later the software was upgraded to VORPAL version 5.2.0 with advanced visualization features. QT Library version 4.8.2 has been configured on this cluster to support advanced visualization features of VORPAL software.

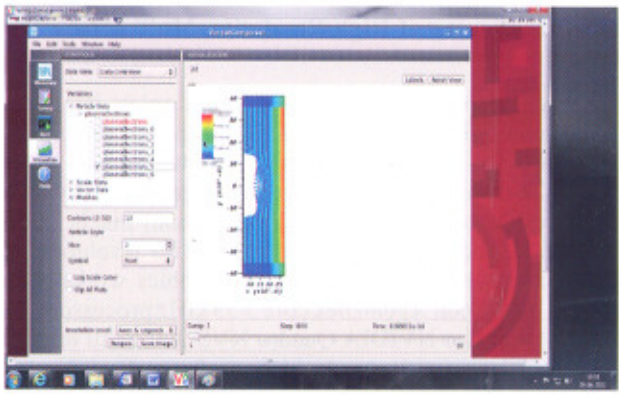

Figure I.1.5: Visualization using VORPAL software

Fiscof software (used for one & two Dimensional Relativistic plasma analysis) and **LPIC,** one-dimensional Particle-In-Cell (PIC) code are ported successfully on Intel Xeon Linux server for Laser Plasma Division.

Urmel is configured and recompiled on Intel Xeon Linux server for RF Systems Division. This software is used to model and simulate the resonance characteristics of a cavity.

Parallel application software **CRYSTAL09** is also successfully ported on HPC cluster Kshitij-2 for Laser Materials Development and Devices Division.

Intel Fortran compiler & OpenMPI version 1.4.2 were used for porting of this software.

Mathematica is successfully installed & configured on Scientific Linux version 6.1 based server.

G) Training and hands-on sessions conducted at User Hall:

Following training and hands-on sessions were conducted at User Hall, Computer Division:

1. XRD Techniques on 27th Jan 2012.
2. Practical Session for TSO between 31st Jan to 2nd Feb, 2012.

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I.2: Development of Information Systems at RRCAT

A) Re-engineering of database structure and code of CAREER and EAGLE software for APAR 2011-12:

Web based software **CAREER**- **C**omprehensive **A**nnual **R**eport **E**valuation with **E**ncrypted storage & **R**etrieval has been re-engineered and appropriate design changes have been made in the database structure to implement new formats introduced for the APAR period 2011-12.

To access year-wise APAR details, the data has been re-organized by maintaining history of employee details to reflect organizational changes and personal information of individual employee for the respective APAR periods. The application software has also been enhanced as per the design changes and enhanced editor has been provided for filing APAR.

Software was modified for filing and assessing APARs for following four different formats:

(i) For all Scientific Officers in the Grade Pay of Rs. 10000 and above

(ii) For all Scientific/Technical Officers in the Grade Pay of Rs. 5400 & up to Grade Pay of `8900

(iii) For Scientific Officers (Medical)

(iv) For Technical Staff from GP Rs. 4800 up to GP Rs. 7600 including SO (B) and TO (B), paramedical staff, Nurses, Pharmacists, etc.

Following two options are provided by the software for filling the APAR by Individual Officer within the time period set by Recruitment Section:

1. Employees can print blank format of 'Part-I : Personal Data', 'Part-II : Self Appraisal' and submit to Reporting Officer after filling them manually.
2. Employees can print APAR 'Part-I : Personal Data' and prepare & print 'Part-II : Self Appraisal' by using the software. Employee can only view their APAR details once they are 'Submitted for Assessment'.

Blank formats of 'Status of accomplishments against tasks/ targets given in previous APAR' and 'Plan of Work for the next year' can be printed and filled manually for submission to Reporting Officer.

Reporting and Reviewing Officers can view the APAR details (Part-I & Part-II) of employees (if submitted online) for whom s/he is Reporting or Reviewing Officer.

EAGLE software – Electronic Assessment Grade Logger and Editor software was re-designed, developed and implemented for assessment, evaluation and printing as per new formats of APAR for 2011-12.

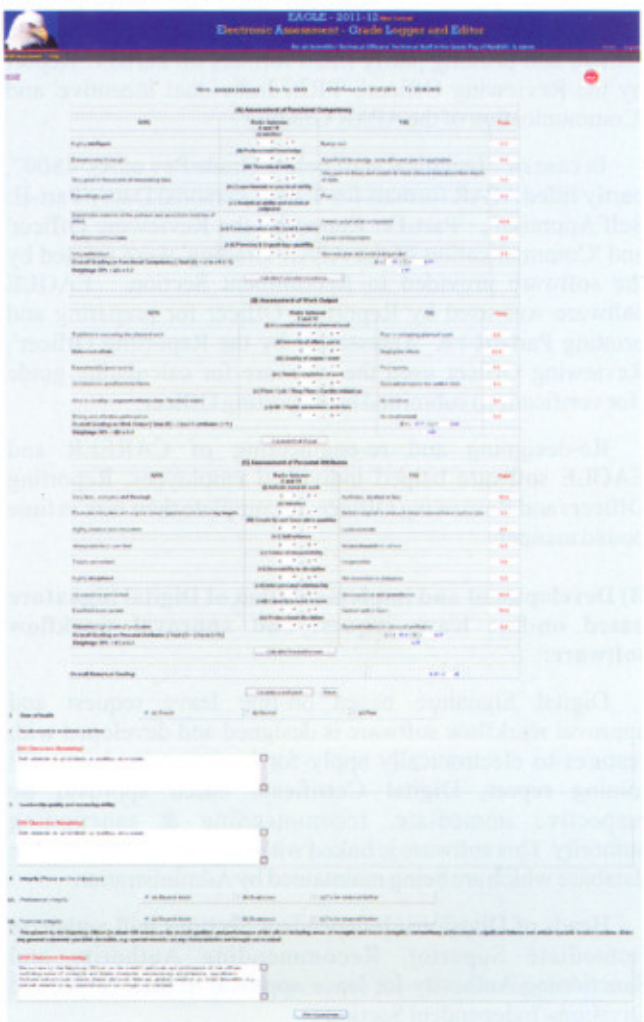

Figure I.2.1: 'Part-III : Assessment by Reporting Officer' for Scientific/ Technical Officers in the Grade Pay of Rs. 5400 & up to Grade Pay of Rs.8900