

## I.1 Scientific Computing and Software Development at RRCAT

### A) Commissioning of High Performance Computing Cluster Kshitij-3 (क्षितिज-3):

High Performance Computing Cluster (HPCC), Kshitij-3 (क्षितिज-3) is commissioned in RRCAT for Scientific and Engineering computing applications. This HPCC is equipped with 64 IBM Blade servers, five Blade enclosures, two IBM rack mounted servers, five numbers of 40 Gbps InfiniBand (IB) switches and one centralized 144 ports 40 Gbps Voltaire IB switch. 768 numbers of computing cores, 6 TB memory and a Storage Area Network (SAN) system for user data storage are also available in Kshitij-3 for advance computations. This cluster delivered Peak Computing Power of 8.5 Teraflops.

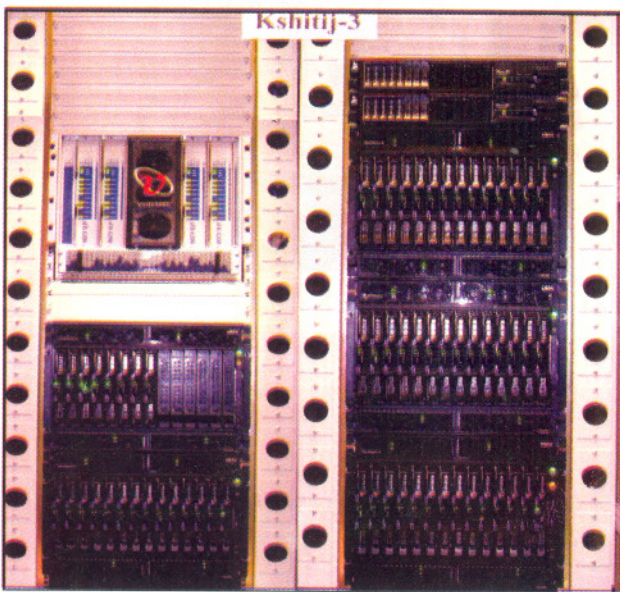


Figure I.1.1: HPC Cluster Kshitij-3

This HPCC has been configured by using Open-source software to function in fail-safe mode. OpenLDAP has been configured in dual master mode and Resource Manager – TORQUE and Scheduler - MAUI are also implemented in high-availability mode. If any problem occurs in master node, cluster will work uninterruptedly with redundant master node.

High I/O capability is one of the main features of this HPCC, which has been implemented through Lustre File System. Lustre version 2.2.0 is configured as file system of Kshitij-3 cluster with QDR InfiniBand Network. Metadata Server (MDS), Object Storage Target (OST), Lustre Network (LNET) and Lustre management server are also installed and configured for implementation of this file system.

Inter Process Communication Libraries - MPICH2 (mpich2-1.5), MVAPICH2 (mvapich2-1.8.1), OPENMPI (openmpi-1.6.3) are configured for supporting various types of parallel applications. Intel FORTRAN & C compilers version 13 and Math Kernel Library are configured on this cluster for parallel computations.

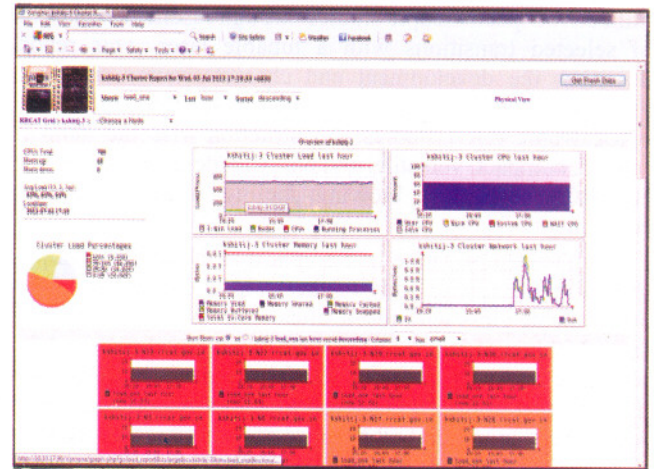


Figure I.1.2: Monitoring of Kshitij-3

Web based scalable distributed monitoring system 'Ganglia' version 3.1.7 has been configured with 'rdtool' version 1.3.8 on Kshitij-3 and deployed on RRCATNet. Consolidated cluster usage in terms of Load, CPU, Memory, Network and detailed usage of each node in terms of Load, CPU, Memory, Network, Disk, Packets in/out etc. are available through this monitoring tool. All these details are available from last one hour to one year in graphical form.

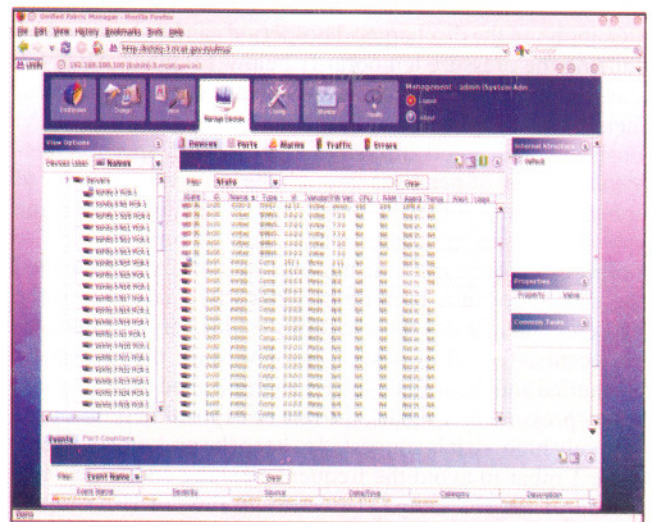


Figure I.1.3: Management of InfiniBand network of Kshitij-3



Unified Fabric Manager (UFM) tool has been installed and configured for management and monitoring of InfiniBand network of Kshitij-3 consisting of 66 numbers of servers, 5 numbers of 18 ports IB switches and one number of centralized 144 ports IB switch. User Interface (UI) of UFM is also implemented for smooth operation of InfiniBand network.

**B) Benchmarking of HPC Cluster Kshitij-3:**

Benchmarking of HPC Cluster, Kshitij-3 was carried out using standard open source Intel MP\_LINPACK and three Inter Process Communication Libraries - MPICH2, MVAPICH2 and OpenMPI.

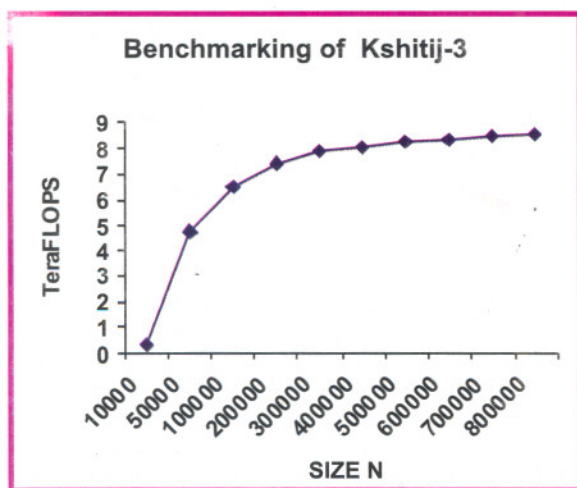


Figure I.1.4: Benchmarking of Kshitij-3 using MVAPICH2

MP\_LINPACK is an implementation of Massively Parallel benchmark by means of HPL (High Performance Linpack Benchmark) code. It solves a random dense (real\*8) system of linear equations (Ax=b) and measures the amount of time it takes to factor and solve the system, converts that time into performance rate and tests the results for accuracy.

Benchmarking tests were carried out with 10,000 as initial size (N) of system of equations and we achieved peak performance of Kshitij-3 cluster at N=8,00,000 as shown in the graph in Figure I.1.4. The peak Computing power (Rmax) of Kshitij-3 is 8.5 Teraflops, which is 90% of theoretical peak performance (Rpeak) of this cluster.

**C) Porting of user programs:**

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

**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-3. This parallel application package bundled with Intel MPI Library has been configured using Intel Fortran compiler and resource manager - TORQUE & scheduler - MAUI. Its windows based portal Material Studio version 6.1 was also configured for submitting jobs on HPC Kshitij-3. This software is used by users from Indus Synchrotrons Utilization Division.

Parallel application **ADF bundle with HPMPI** (Amsterdam Density Functional, version 2013 - a FORTRAN program for calculations on atoms and molecules) has been successfully ported and tested through resource manager - TORQUE & scheduler - MAUI on Kshitij-3. This parallel application is used by users from Indus Synchrotrons Utilization Division

The three-dimensional particle-in-cell (**PIC**) code VLPL (Virtual Laser Plasma Lab - which allows direct fully electromagnetic simulations of relativistic laser-plasma interactions) has been ported successfully on Kshitij-3 HPCC using MVAPICH2 version 1.8.1 and Intel Compilers. This parallel application is used by users from Laser Plasma Division.

Sequential version of **GROMACS** (versatile package to perform molecular dynamics - simulate the Newtonian equations of motion for systems with hundreds to millions of particles) has been successfully ported on Linux based computing server with graphical user interface. This software is used by users from Laser Biomedical Applications & Instrumentation Division.

Sequential application, **EGSnrc** (NRC's electron gamma shower (EGS) software tool - used to address a broad range of questions about the propagation of radiation in materials) has been ported successfully on Linux based computing server and used by users from Indus Operations and Accelerator Physics - Design Division.

Sequential version of **Multi** (computer program that simulates behavior of the matter at high densities of energy typically found in Inertial Fusion Energy (IFE) and in related experiments of laser interaction with matter) and Medusa (One-dimensional Lagrangian hydrodynamic code) have been successfully ported and tested on Linux based computing server. GNU C compiler version 4.1.2 and X11 library are used to port these software packages, which are used by users from Laser Plasma Division.

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