

I.1 Scientific Computing and Software Development at RRCAT

A) HPC cluster Kshitij-2 (क्षितिज-2):

Blade server based High Performance Computing (HPC) Linux cluster comprising of 64 Quad Core Xeon Processors/ 256 cores, with aggregate memory of 2 Terabytes has been commissioned for advanced computing applications. The cluster named Kshitij-2 (क्षितिज-2) is commissioned with high-end 40 Gbps InfiniBand interconnect and high capacity Storage Array (HP EVA 6400). All nodes of this cluster are HP BL460c G6 series blade servers and the cluster is built using open source software packages. The cluster delivered Peak Computing Power of 2.82 Teraflops.

High capacity storage array (HP EVA 6400) of HPC cluster kshitij-2 has been configured in failover mode. We have used HP Device Mapper Multipath (HPDM Multipath) tool to connect dual controller based high capacity storage array with Kshitij-2 cluster.

Inter Process Communication Libraries - MPICH2 (mpich2-1.3.2), MVAPICH (mvapich-1.2.0), MVAPICH2 (mvapich2-1.5.1), OPENMPI (openmpi-1.4.2) are configured for supporting advanced and also backward compatibility with Inter Process Communication (MPI) Libraries. Math Kernel Library, SCALAPACK, ATLAS are also configured along with compilers like Intel Fortran and C, GNU Fortran and C for sequential and parallel applications.

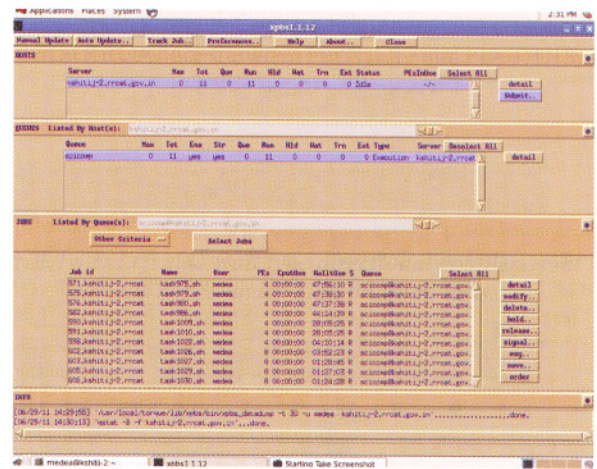


Fig. I.1.2: GUI of TORQUE in Kshitij-2.

Web based, scalable, distributed monitoring system 'Ganglia' version 3.1.7 has been configured with 'rrdtool' version 1.3.7 on Kshitij-2 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. is available in this monitoring tool. All these details are available from last one hour to one year in graphical form.

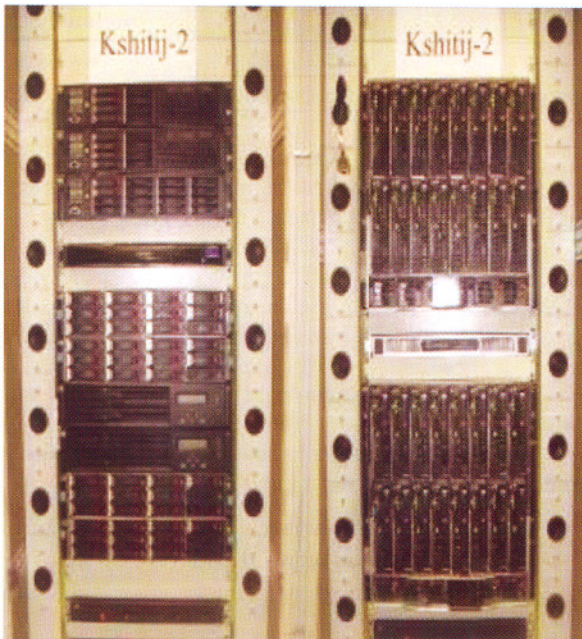


Fig. I.1.1: HPC cluster Kshitij-2.

This HPC cluster is configured using open source resource manager TORQUE (torque-3.0.0) and open source advanced scheduler MAUI (maui-3.3). Resource manager starts, holds, cancels & monitors jobs running on the cluster. Scheduler works with resource manager to maximize output of the cluster. TORQUE is configured with GUI and users can manage their jobs with this GUI.



Fig. I.1.3: Monitoring of Kshitij-2.



B) Benchmarking of HPC cluster Kshitij-2:

Benchmarking of Kshitij-2 has been carried out using Intel optimized MP LINPACK Benchmark for clusters, which is an implementation of Massively Parallel MP LINPACK 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.

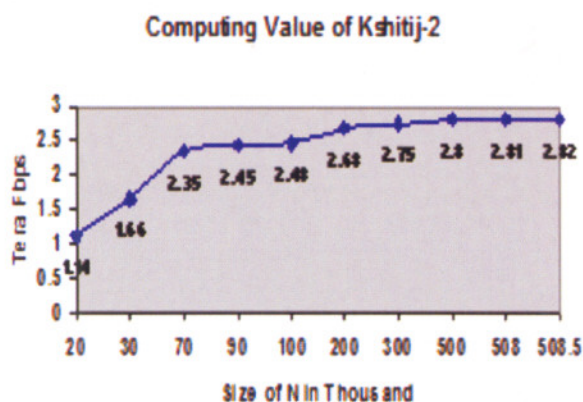


Fig. I.1.4: MP LINPACK graph of Kshitij-2.

Benchmarking tests were carried out with 20,000 as initial size (N) of system of equations and we achieved peak performance of Kshitij-2 cluster at N=508500 as shown in MP LINPACK graph shown in Figure I.1.4. The peak performance of Kshitij-2 is 2.82 Teraflops, which is 93% of theoretical peak performance (Rpeak) of this cluster.

C) Augmentation in DAEGrid:

DAEGrid is operational in BARC, RRCAT, IGCAR, and VECC to share computing resources. For better use of DAEGrid resources, grid middleware of Ramanujam & Daksha clusters and User Interface machine has been changed from gLite3.1 to gLite3.2. Operating System is also upgraded to Scientific Linux 5.5 on both clusters and User Interface machine. Intel Fortran version 11, gcc, gfortran, parallel processing libraries mpich2-1.1 and mpich-1.2.7 are installed on both of these clusters. Users of DAEGrid can submit their sequential and parallel applications on both these clusters.

D) Porting of user programs:

As per requirement of users, various software packages have been successfully ported or upgraded on computing servers and clusters.

Parallel software packages VASP (Vienna Ab-initio Simulation Package - a package for performing ab-initio quantum mechanical molecular dynamics using either Vanderbilt pseudo potentials, or the Projector Augmented Wave Method, and a plane wave basis set) is successfully ported on Kshitij-1 and Kshitij-2 clusters. This code is being used by scientists of Indus Synchrotrons Utilization Division and Laser Physics Applications Division.

Parallel application packages ORBIT_MPI (Objective Ring Beam Injection and Tracking - a particle tracking code for particle accelerator rings) is successfully ported on Aryabhata cluster using GNU FORTRAN 77 & C (g77, gcc) compiler, MPICH version 1.2.7, FFTW version 2.1.5. Porting of this software was required by Indus Operations & Accelerator Physics Design Division.

Parallel application software SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms - is an original method and a software implementation for performing electronic structure calculations and ab-initio molecular dynamics simulations of molecules and solids) is successfully ported on Kshitij-1 & Kshitij-2 clusters using OpenMPI, Intel FORTRAN compiler version 11 and Intel Math Kernel Library. This code is being used by users from Indus Synchrotrons Utilization Division.

Particle physics MonteCarlo simulation package, FLUKA has been upgraded from version 0.7 to version 0.9 and its graphical user interface, FLAIR is also upgraded from 2008.3c-0 to version 2008.3d.1 on Linux based computing server. This software is used regularly by users from Industrial & Medical Accelerator Section and Indus Operations & Accelerator Physics Design Division.

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

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

1. ANSYS software version 13 on 9th Feb. 2011.
2. Microsoft Excel during March 7-11, 2011.
3. E-Tender software during March 22-25, 2011.
4. SIMPLORER software during May 5-6, 2011.
5. Exceed software on 26th May 2011.

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