

I.1 Scientific Computing and Software Development at RRCAT

A) Teraflop HPC cluster Kshitij-1 (क्षितिज -1):

Blade server based High Performance Computing (HPC) Linux cluster comprising of 32 Quad Core Xeon Processors/ 128 cores with aggregate memory of 512 GB has been commissioned for scientific computing applications. The cluster named Kshitij-1 (क्षितिज -1) is commissioned with high-end 20 Gbps InfiniBand interconnect and high capacity Storage Array (HP EVA 4400). All nodes of this cluster are HP BL460c series blade servers and cluster is built using open source software packages.

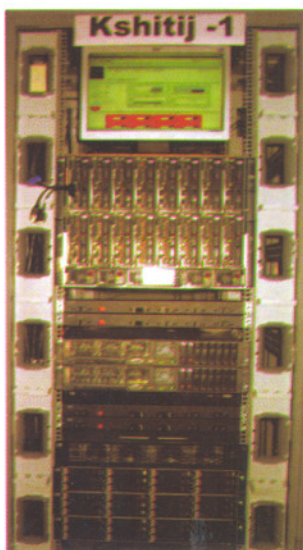


Fig. I.1.1: HPC cluster Kshitij-1.

The cluster is benchmarked by us using standard open source Intel MP_LINPACK (Implementation of Massively Parallel MP LINPACK benchmark by means of HPL code) and it delivers Peak Computing Power of 1.26 Teraflops.

This HPC cluster is configured using open source resource manager TORQUE (torque-2.4.0b1) and open source advanced scheduler MAUI (maui-3.2.6p21). Open source cluster monitoring tool Ganglia-3.0.4 is also configured on this cluster.

Many Open source parallel processing libraries like MPICH2 (mpich2-1.0.5), MVAPICH (mvapich-1.1), MVAPICH2 (mvapich2-1.2p1), OPENMPI (openmpi-1.3.3) are configured for supporting advanced features and also to provide backward compatibility with parallel processing (MPI) libraries. Math Kernel Library LAPACK, ATLAS are

configured along with compilers like Intel Fortran and C, GNU Fortran and C for sequential and parallel applications.



Fig. I.1.2: Monitoring of Kshitij-1.

B) Mathematica version 7:

Computational and engineering software tool Mathematica has been upgraded to latest version (version 7) with five users network floating licenses. The software tool has been configured on Intel based Linux server. Mathematica version 7 supports built-in Digital Image Processing & Analysis, built-in Parallel Computing, Automated Charting Graphics, Industrial-Strength Boolean Computation, New Number Theory Capabilities, Integer Sequence Analysis, Enhanced Fourier Analysis and various other new features. Three days training with hands-on was also organized for Mathematica users at User Hall, Computer Centre.

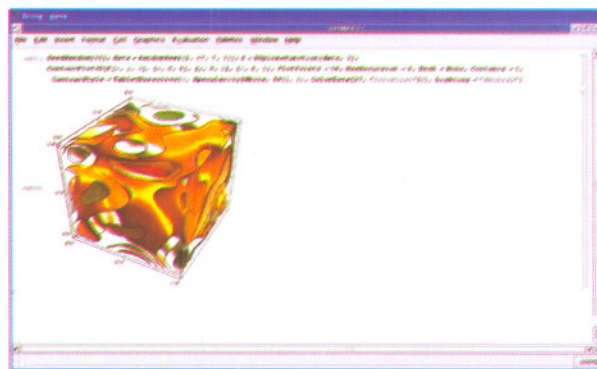


Fig. I.1.3: Using Mathematica7 from Remote Windows desktop.

C) Speed-up analysis of MPI variants on cluster with InfiniBand interconnect:

High performance computing systems have a trend towards distributed memory architecture with high speed

interconnects like Myrinet, Quadrics, Gigabit Ethernet and InfiniBand. MPI standards are widely used in distributed memory systems. We have carried out performance analysis of MVAPICH (MVAPICH2 and MVAPICH) and Open MPI to analyze suitability of different MPI standards over InfiniBand interconnect using Intel MP_LINPACK open source software. The graph below shows the results obtained.

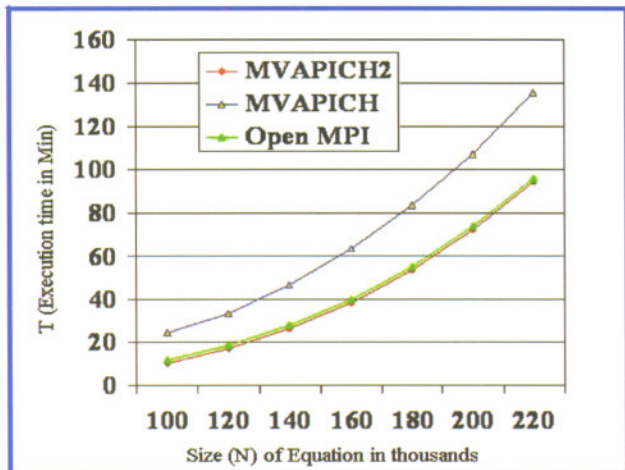


Fig. 1.1.4: Performance of MVAPICH2, MVAPICH and Open MPI with InfiniBand interconnect.

Results of tests carried out for different sizes of system equations revealed that MVAPICH2 delivers better performance as compared to Open MPI and MVAPICH. Thus applications should be based on MVAPICH2 variant of MPI if they are intended to run on high performance computing cluster with InfiniBand interconnect.

D) Porting of user programs:

As per requirement of users, various software packages were successfully ported on computing servers and clusters. GUI based Biological Application software Autodock version 4.0 has been successfully ported on Intel Itanium2 based Linux platform. This application has been configured with GUI MGLTools version 1.5.4, Python-2.5, tcl/tk-8.4 and Swig-1.3.31. The sequential applications successfully ported are: CST STUDIO SUITE 2008, Flair (Fluka Advanced Interface) version 0.7, MELD & PPP on Intel Xeon based Linux servers.

The parallel applications successfully ported on Kshiti-1 cluster are: ADF-2009 bundle with HPMPI (Amsterdam Density Functional, version 2009 - a FORTRAN program for calculations on atoms and molecules) and CPMD (Car-Parrinello Molecular Dynamics - Electronic Structure and Molecular Dynamics Program).

E) Centralized access of ANSYS-12:

ANSYS-12 has been installed and configured on Intel Itanium2 based high-end server Ganak-1 with X11 and OpenGL (Open Graphics Library) for 2D & 3D graphics. All ANSYS users can access ANSYS-12 software by connecting Ganak-1 server through remote graphical display from their Windows and Linux desktops using X Display Manager Protocol (XDMCP).

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I.2: Development of Information Systems at RRCAT

A) Migration of client/ server based Medical Centre Information Management Software (Chikitsa) to web based architecture:

Medical Centre Information Management Software (Chikitsa) has been migrated to web based platform using n-tier architecture, earlier it was running on two-tier client/ server architecture. Xeon based Oracle 10g Database Server and Application Server were installed and configured for authentication from Oracle Internet Directory. Migration and re-engineering of data from Oracle 7.3 to Oracle 10g was carried out while maintaining data integrity and consistency. Migration of forms and reports using Oracle Developer Suite 10g, application deployment on Application Server 10g and unified login was completed with single sign-on functionality.

Re-structuring of the software and database was done to overcome shortcomings of earlier software. New features were added for annual stock taking and report generation from

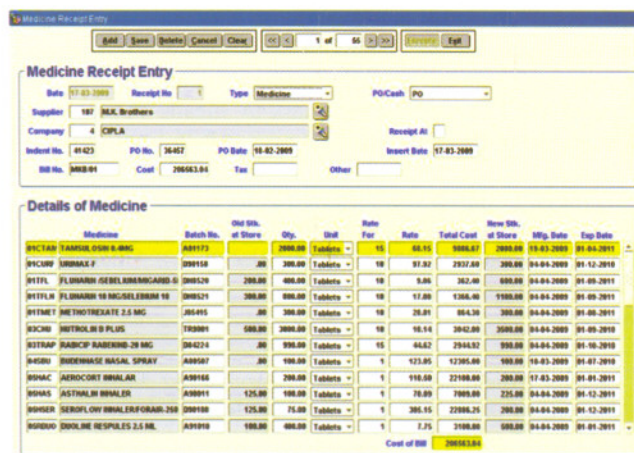


Fig. 1.2.1: Snap shot showing entry of received medicines.