

I.1 Scientific Computing and Software Development at RRCAT

A) Commissioning of Centralized and Redundant Storage Area Network for High Performance Computing Clusters:

Centralized Storage Area Network (SAN) based on high bandwidth fiber channel connectivity is devised and commissioned for High Performance Computing Clusters: Kshitij-1 (क्षितिज-1), Kshitij-2 (क्षितिज-2) and Kshitij-3 (क्षितिज-3) and it is now operating in redundant mode. Two HP Storage Works 8/24 SAN switches and two Brocade 4/24 SAN switches are used to build this redundant SAN Network as shown in figure I.1.1.

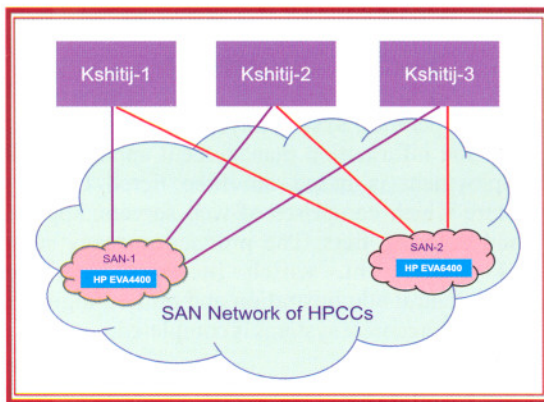


Figure I.1.1: Redundant SAN Connectivity for HPCCs

Using this setup, reliability of important user data on clusters is increased. In addition, user area has also been increased using this redundant SAN network. User data area of Kshitij-2 cluster is increased from 4 TB to 8 TB. Both storage arrays HP EVA 4400 and HP EVA 6400, each with raw capacity of 12 Terabytes, are connected to the clusters through this storage network. One storage array is used to provide file services for important user data and other storage array is used for backup of user data. This setup has been devised in such a way that availability of user data is ensured in case of failure of any one of the storage arrays.

B) Testing and performance evaluation of ANSYS Fluent HPC software on Kshitij-3 cluster:

Testing and performance evaluation of ANSYS Fluent HPC software has been completed successfully on Kshitij-3 cluster. ANSYS Fluent HPC software and its benchmark programs were ported using OPENMPI version 1.6.3. Scripts were developed to submit jobs using resource manager TORQUE. This parallel application has been tested using 32 and 128 number of cores of Kshitij-3 cluster. Three benchmark cases: eddy_417K, sedan_4M and Truck_14M

were tested on Kshitij-3 cluster using 24 cores, 32 cores, 48 cores and 128 cores. Performance of these benchmark cases on Kshitij-3 cluster is very encouraging indicating that this cluster is highly suitable for running such engineering applications.

C) Modifications and porting of EPOCH software

Parallel application **EPOCH versions 4.2.5 and 4.2.11 (Extendable PIC Open Collaboration** - a multi-dimensional, fully electromagnetic, relativistic particle-in-cell code) is an open source software developed in FORTRAN for plasma physics simulation. Both the versions of this parallel application, originally execute in interactive mode. This parallel FORTRAN code has been modified to function in non-interactive mode and also to accept all inputs as command line parameters.

EPOCH software generates large files at the time of execution and typical size of file is more than 20 GB. The code has been modified for exception handling in case of file Read and Write operations. The modified software is ported successfully on HPC cluster Kshitij-3 using Intel FORTRAN version 13 and OPENMPI version 1.6.3. This parallel application is used by users of Laser Plasma Division at RRCAT.

E) Porting of user programs:

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

Parallel application named WIEN2K_12 (Computation of electronic structure of solids within density functional using Linearized Augmented Plane Wave (LAPW) method) is successfully ported on HPC cluster Kshitij-2, using Intel FORTRAN compiler version 11 and OPENMPI version 1.4.2. This application is also successfully tested through resource manager, TORQUE and scheduler, MAUI.

Parallel application named SPRKKR (Spin-Polarized Relativistic KKR band structure program package) is successfully ported on Kshitij-3 HPC cluster using Intel FORTRAN compiler version 13 and OPENMPI version 1.6.3. The application is successfully tested through resource manager, TORQUE and scheduler, MAUI.

WIEN2K_12 & SPRKKR are used by users of Indus Synchrotrons Utilization Division at RRCAT.

Parallel application software named **CRYSTAL09**, is ported successfully on HPC cluster Kshitij-3 for users of Laser Materials Development and Devices Division at RRCAT.



Intel FORTRAN compiler version 13 & OPENMPI version 1.6.3 were used for porting of this software.

VisIt version 2.6.3 (distributed, parallel, visualization tool for visualizing data defined on two- and three-dimensional structured and unstructured meshes) is successfully ported on Kshitij-3 cluster using Visualization Toolkit (VTK) version 6.0.0. This visualization tool is used to visualize large simulation data at its place of generation, thus eliminating the need to move the voluminous data to other visualization server.

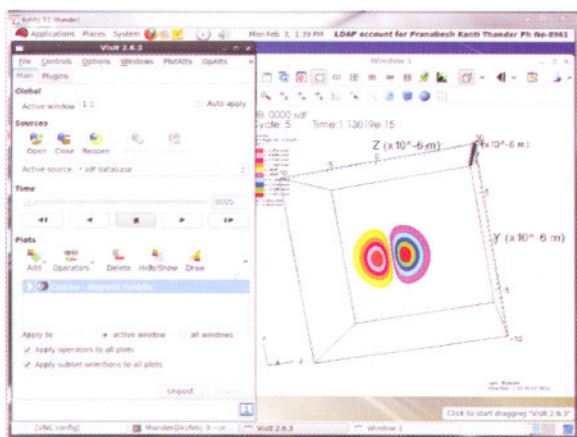


Figure I.1.2: 3D Visualization of output data of EPOCH using VisIt

VisIt tool is used by users of Laser Plasma Division of RRCAT, to visualize output of **VORPAL** and **EPOCH** parallel applications.

GDL version 0.9.3 (GNU Data Language) is successfully installed and configured on Kshitij-3 cluster for users of Laser Plasma Division at RRCAT, for visualization based analysis of output.

XCRYSDEN version 1.5.53 (crystalline and molecular structure visualization program) is successfully installed and configured on Kshitij-2 cluster to visualize and analyze output generated by parallel applications **CRYSTAL 09** and **Quantum ESPRESSO**. This tool is used by users of Laser Materials Development and Devices Division, Indus Synchrotrons Utilization Division and BARC Training School at RRCAT.

In addition to porting of application programs, license of ANSYS multi-physics version installed in Computer Centre, has been upgraded to version 14.5 and license of Material Studio version 6.1 is also installed on HPC cluster Kshitij-3.

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I.2: Development of Information Management Systems at RRCAT

A) Commissioning of Oracle 11g platform for next generation of Information Management Systems:

Various information management systems being used in RRCAT Administration, Accounts, IRPSU and Medical centre, are deployed on Oracle 10g platform and are operational since year 2007. These applications and associated databases are required to be migrated to Oracle 11g platform, since support for Oracle 10g Database and Application server Release 2, expired in July 2010 and Oracle 10g setup is not compatible with latest server hardware. Also, the old version of Application Server supports only JDK (Java Development Kit) 1.3, which is also an un-supported version.

Intel Xeon based **HP enterprise** servers with 32 GB memory, 3.6 TB storage and open source Enterprise Linux release 5.7 as Operating System have been commissioned for next generation information management applications. The server deployment is based on three tiered Oracle 11g infrastructure which comprises of web servers, application servers and database tiers. The production ready setup of Oracle 11g platform, which includes, application deployment, central administration and unified login across information management systems is completed.

Installation and commissioning of NAS (Network Attached Storage) based backup solution for performing backup of data on database servers, application software and system software repository was completed. Two numbers of NAS devices, having two Intel Xeon Processors of 2.26 GHz, 24 GB memory and 28 TB storage capacity with Windows 2012 storage server as underlying Operating System, have been installed. These two NAS devices are used for offline backup of Oracle 10g/ Oracle 11g database and software code on Oracle 10g/Oracle Web logic application server.

B) Migration and re-engineering of Integrated Purchase-Stores-Audit Software and OASIS Software to Oracle 11g platform:

Migration of data from Oracle 10g database to Oracle 11g database was completed for Integrated Purchase-Stores-Audit Software and Project Monitoring Software - OASIS. Application porting and re-engineering of forms and reports on Oracle 11g Web logic mid-tier, was completed. Now, Integrated Purchase-Stores-Audit Software and OASIS Software both are successfully running on Oracle 11g platform with Oracle Single Sign-on functionality. The whole exercise has resulted in a sustainable information system which is compliant with international standards.