

I.1 Scientific Computing and Software Development at RRCAT

A) Augmentation of Centralized Computing Server Setup:

Computing server named as Amogh-6 (अमोघ-6) has been commissioned with two Intel Xeon 2.93 GHz hex core processors & 16 GB memory for scientific computing and engineering applications. Red Hat Enterprise Linux Server release 5.5 is used as operating system for this server. Intel C & FORTRAN compilers version 11.1 and Math Kernel Library version 11 are configured for advanced computing and engineering applications.

LAPACK (Linear Algebra PACKage) and ATLAS (Automatically Tuned Linear Algebra Software) are also installed on this server. Qt (cross platform GUI toolkit version 4.3.4), 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 on this server for latest GUI based scientific & engineering applications.

B) Enhancement of Virtual Cluster Setup for OPERA Software:

Virtual Cluster Setup being used for OPERA Software has been upgraded to support more computing requirement. Memory of two servers is upgraded to 32 GB each, and user areas are also upgraded to 800 GB on both the servers. Memory and user area on License server of this software are also upgraded to 16 GB and 800 GB respectively. With augmentation of hardware resources, execution speed of Opera software has increased significantly and users have more area to save their data.

C) Augmentation in DAEGrid:

Storage Element (SE) of DAEGrid has been upgraded to support grid middleware - glite-3.2. Operating System of SE server is also upgraded to Scientific Linux release 5.5. LCG Disk Pool Manager has been configured on this 64-bit Scientific Linux based Storage Server, which is functioning with catalogue services of DAEGrid. RRCAT users as well as users on DAEGrid can store huge files on this server, which is essential for computing applications.

D) Porting of user programs:

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

ASTER version 10.0.3 is ported successfully on Intel Xeon Linux server. This software is a general code directed at the study of the mechanical behaviour of structures including thermal and mechanical non linear analysis.

SALOME version 6.3.1 is ported on Intel Xeon Linux server. SALOME is free software that provides a generic platform for Pre and Post-Processing for numerical simulation. SALOME platform supports interoperability between CAD modeling and computation software (CAD-CAE link).

ELMERFEM is successfully ported on Intel Xeon Linux server. ELMER is an open source GNU General Public License (GPL) computational tool for multi-physics problems. ELMER includes physical models of fluid dynamics, structural mechanics, electromagnetics, heat transfer and acoustics. These are described by partial differential equations, which ELMER solves by the Finite Element Method (FEM). ELMER comprises of several different modules: The boundary conditions and physical models are defined in ElmerGUI. The resulting problem definition is solved by ElmerSolver. Finally the results are visualized by ElmerPost. Additionally, a utility ElmerGrid may be used for simple mesh manipulation.

Porting of above three software packages, ASTER, SALOME and ELMERFEM was required by Laser Material Processing Division.

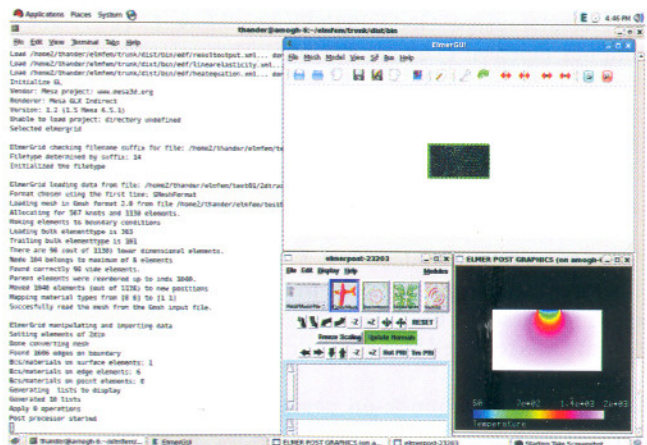


Figure I.1.1: Computation and plotting using ElmerGUI, ElmerSolver, ElmerPost

Elegant software is also successfully ported on Intel Xeon Linux server. Elegant (ELEtron Generation ANd Tracking) is a tracking code. Its capabilities include six dimensional tracking using matrices up to third order, canonical integration, and numerical integration. Elegant can optimize a user defined function of the transfer matrix



elements (up to third-order), beta functions, tunes, chromaticities, radiation integrals, natural emittance, floor coordinates, beam moments, etc.. It also has the ability to optimize results of tracking using a user-supplied function of the beam parameters at one or more locations.

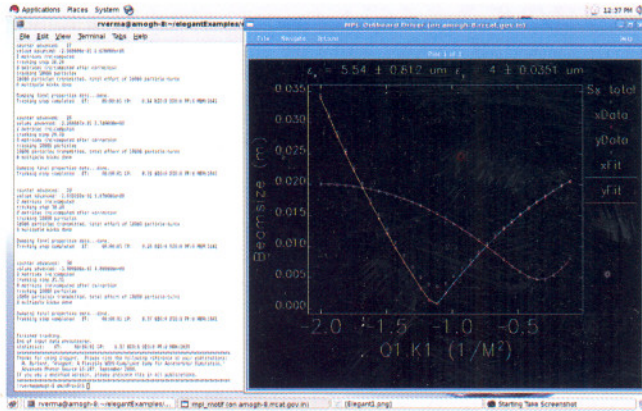


Figure I.1.2: Beam analysis using Elegant and its GUI

Sequential application **Tracy3** is successfully ported on Intel Xeon Linux server. This program does the computation of off momentum particle (i.e. electrons) loss in presence of multipolar magnetic field error.

Parallel application **ORBIT_MPI** (Objective Ring Beam Injection and Tracking - a particle tracking code for particle accelerator rings) is successfully ported on Kshitij-1 HPC cluster using GNU FORTRAN 77 & C (g77, gcc) compiler, OpenMPI version 1.3.3, FFTW version 2.1.5.

Porting of above three software packages i.e. Elegant, Tracy3 and ORBIT_MPI was required by Indus Operations & Accelerator Physics Design Division.

Parallel application **ADF** bundle with HPMPI (Amsterdam Density Functional, version 2010 - a FORTRAN program for calculations on atoms and molecules) has been ported successfully on Kshitij-2 HPC cluster. Porting of this software was required by SRS Coordination section.

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

One week training course on **Microsoft Excel** was organized by Computer Centre for RRCAT employees in two batches during 18th July to 29th July 2011.

One week training course on **HTML 5** was organized by Computer Centre from 10th October to 14th October 2011.

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I.2: Development of Information Systems at RRCAT

A) Commissioning of new RRCATInfonet server in load balancing mode for high availability of applications:

The reliability and availability of RRCATInfonet server has become critical due to deployment and wide usage of applications like Project Monitoring Software, Budget Monitoring Software, Indent Preparation Module, Purchase Information Module, software packages for APAR (Annual Performance Assessment Report) Evaluation and Assessment, Leave, Payslip & Income Tax details etc.. These application software packages have wide user base, thus they have direct performance value and time window limit associated for any downtime and unavailability.

Server Load Balancer SLB was installed and configured for Tomcat web server with features for application acceleration, failover, security and management for new RRCATInfonet clustered servers.

The new setup of Server Load Balancer and clustered web server has been configured to provide high performance, high availability, and scalability of RRCATInfonet applications by distributing the load among application servers. Load balancing switch has been configured to route the http, https, sftp and smtp requests to distribute load among application servers by maintaining IP persistency in round-robin manner. Two Application servers have been setup by using Apache Tomcat v 6.0.29 and JRE v 1.5. One server has been configured as file server to share the application directory to the web servers over NFS (Network File System version 4.0).

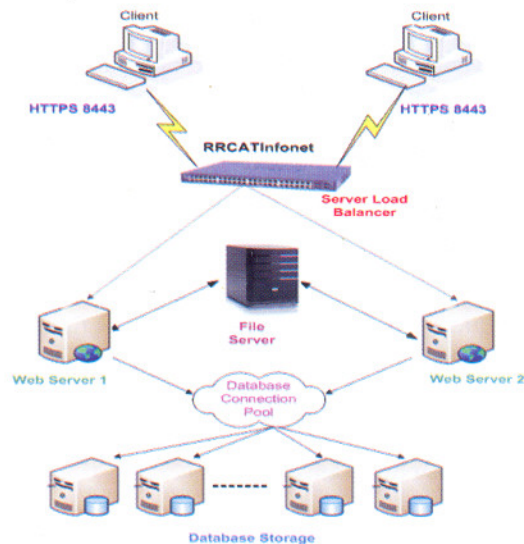


Figure I.2.1: Server Load Balancer for applications on RRCATInfonet