I.1: Scientific Computing and Software Development at RRCAT

A) Centralized access of MATLAB software:

MATLAB 7.10.0 (R2010a) has been installed as centralized facility with two network floating licenses. MATLAB software provides a high-level programming language, an interactive technical computing environment, functions for algorithm development, data analysis and visualization.

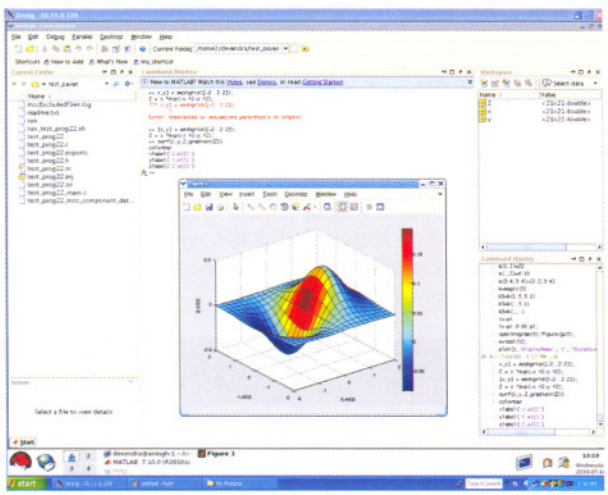

Fig. I.1.1: 3-D Visualization with Coloring Mesh & Surface plots using MATLAB

The installed software package includes many modules and toolboxes in addition to the core package and MATLAB compiler. Various toolboxes are - Partial Differential Equation, Optimization, Statistics, Curve Fitting, Spline, Signal Processing, Symbolic Math, Genetic Algorithm and Direct Search, Parallel Computing.

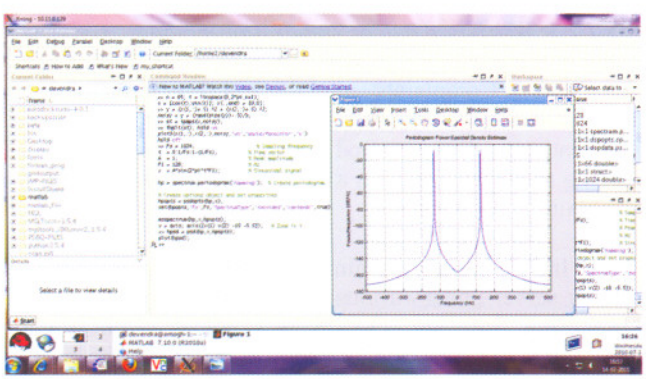

Fig. I.1.2: Measuring Signal Power in Spectral Analysis using Signal Processing Toolbox in MATLAB

MATLAB and its licenses are installed on Intel based Red Hat Enterprise Linux 5 server with two Xeon quad core 2.93 GHz processors and 16 GB memory. Users can access MATLAB from their Windows/ Linux desktop with OpenGL (Open Graphics Library) for 2D & 3D graphics support.

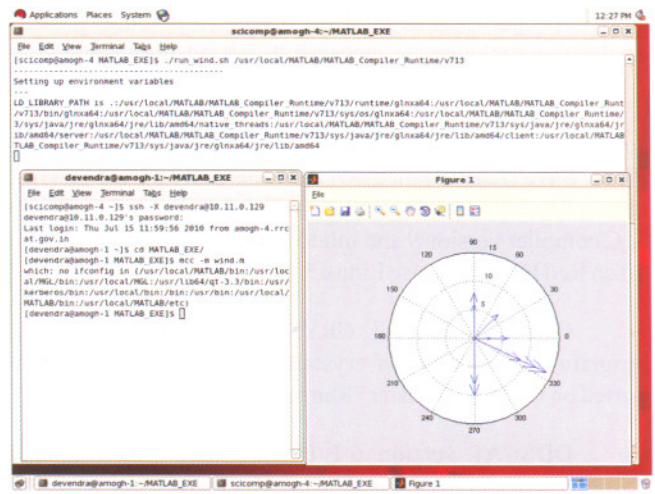

Fig. I.1.3: Running executable using MCR

MATLAB Compiler Runtime (MCR) facility is also made available for RRCAT scientists. MCR is a set of shared libraries that enable the execution of MATLAB files on computers without an installed version of MATLAB and MCR works in both Windows and Linux environments.

B) Setup of storage in failover mode for Kshitij-1 cluster:

High capacity storage array (HP EVA 4400) of HPC cluster Kshitij-1 has been configured in failover mode. HP Device Mapper Multipath (HPDM Multipath) tool is used to connect dual controller based high capacity storage array with the cluster in failover mode.

C) Installation of new license server:

Various commercial software packages procured by users require centralized license server to provide network licenses for running application on client machines. An entry level server with Intel Xeon processor has been configured as license server with operating system Red Hat Enterprise Linux 5. The licenses of LS-DYNA version 971 and ANSYS-12 are configured on this server.

D) Backup of computing servers:

Backup mechanism of user area of NIS based computing servers has been configured using centralized SAN based Tape Library backup system of Computer Centre. LTO-4 tape drives are supported by this high speed data

backup system. Red Hat Enterprise Linux 5 based portal has been configured and backup of user area of computing servers is scheduled through this portal.

E) Porting of user programs:

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

WIEN2K_08 [computation of electronic structure of solids within density functional using Linearized Augmented Plane Wave (LAPW) method] is successfully ported on HPC cluster "Kshitij-1" using OPENMPI-1.3.3, Intel FORTRAN & C compiler version 9 and Intel Math Kernel Library version 10 on Red Hat Enterprise Linux 5.

CRYSTAL06 and CRYSTAL09 (General-purpose program for the study of crystalline solids) is successfully ported on DAEGrid cluster "Ramanujam".

DDSCAT version 6.1 (to calculate scattering and absorption of electromagnetic waves by targets with arbitrary geometries and complex refractive index using discrete dipole approximation) is successfully ported on HPC Cluster "Aryabhatta" using MPICH2-1.0.5.

F) Electronic bulletin board:

Status monitoring of various activities is displayed on a plasma TV in Computer Centre. It is a web based presentation to display static and dynamic contents. It displays monitoring status of various clusters and usage of leased links dynamically in addition to static information like activities of Computer Centre, RRCAT web pages etc.

G) Training and hands-on sessions conducted in User Hall:

Workshop on "Extended X-Ray Absorption Fine Structure (EXAFS)" was conducted by Indus Synchrotrons Utilization Division on 9th March 2010.

Training with hands-on session on "MATLAB" was organized by Computer Centre from 17th May to 21st May 2010.

Training with hands-on was conducted by Computer Centre on "Microsoft Office Excel" for staff of Administration and Accounts from 31st May to 12th June 2010.

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I.2: Development of Information Systems at RRCAT

A) Enhancements to RRCATInfonet:

Various new features were added to RRCATInfonet, which include Indent preparation module, Civil Complaints module, Conference Management Software, Indus Operation Training manuals etc.

Web based Indent Preparation module along with Annexure loading can be accessed by indenting officers and division/ section offices after authentication. This module will help in reducing the data entry work related to indent preparation at IRPU, as the data will be entered electronically by indentor on RRCATInfonet. After receiving signed copy of indent, the staff in IRPU will transfer the data from RRCATInfonet server to IRPSU server for further processing. Annexure details can also be uploaded on the server for future reference. Storage of annexure details will help IRPU staff significantly while preparing the purchase orders by avoiding duplicate data entry work.

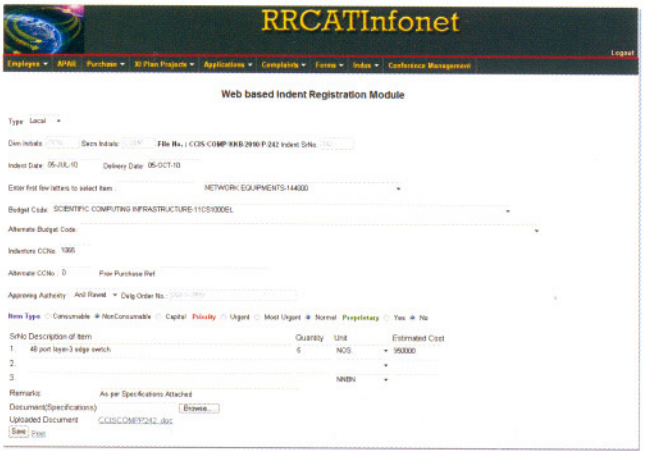

Fig. I.2.1: Web based Indent Preparation module

Civil Complaints module has been released for logging civil, water supply and sewerage related complaints. Automatic email is generated to the concerned authority after logging the complaint with a copy to the person logging the complaint.

Indus Operation Training Manuals were uploaded on Infonet server under various levels in PDF format. Project Monitoring Software, OASIS was enhanced to provide information based on categorization of indents on the basis of PO value. Option for printing month-wise list of certified telephone bills (Telephone Register) by the employees has also been added on RRCATInfonet.