I.1 Scientific Computing and Software Development at RRCAT

A) Storage Server for DAEGrid:

DAEGrid is operational in BARC, RRCAT, IGCAR, and VECC to share computing resources. Storage server of 1.6 TB capacity has been commissioned as part of DAEGrid and it can be accessed through DAEGrid portal and clusters.

LCG Disk Pool Manager has been configured on this 64-bit Scientific Linux based Storage Server. The server 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.

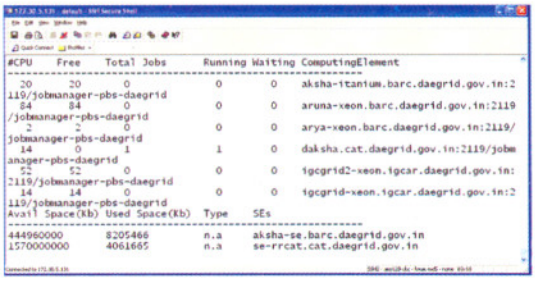

Fig. I.1.1: Typical listing of DAEGrid resources.

B) Augmentation of High Performance Computing Cluster 'Aryabhatta':

The high performance computing cluster, 'Aryabhatta' has been augmented to have 64 processors (128 cores) and 256 GB memory to meet enhanced computing requirements of computing users. 450 gigaflops of peak computing power (benchmarking through MP_LINPACK) has been achieved on this cluster. Redundant file server has been configured for this cluster.

C) High availability File Servers:

File Servers of NIS based computing setup have been upgraded to provide high speed data access along with high-availability feature. The access speed is doubled as compared to earlier setup. Two number of HP ML 370 G5 Xeon based Linux servers with RAID 5+0 are configured in hot-standby mode to provide high speed file access and data redundancy. Storage capacity for computing user's area is enhanced to 860 GB.

D) Scientific Libraries:

CERNLIB - CERN Program Library has been configured on 32-bit and 64-bit Linux based computing servers and made available for computing uses. To meet enhanced requirement of computing applications, parallel MPI library- MPICH-1.2.7, Math kernel Library (version 8), Intel Fortran and C compilers are configured on all seven worker nodes of 'Daksha' cluster of DAEGrid.

E) Porting of user programs:

As per requirement of users, various software packages were successfully ported on computing servers and clusters.

The programs successfully ported on Intel based servers were: Energy Gain of Photoelectrons (computes the energy gain of an initially stationary electron due to the passage of a positively charged bunch, as a function of radius of the electron in the beam pipe), ECLOUD (simulates the build up of an electron cloud, which occurs due to photoemission and secondary emission inside an accelerator beam pipe during the passage of a narrowly spaced proton or positron bunch train). CPMD (Car-Parrinello Molecular Dynamics - Electronic Structure and Molecular Dynamics Program) and WIEN97 were successfully ported on IBM Power 5+ RISC architecture.
The programs successfully ported on clusters were: Parallel application CPMD on 'Daksha' cluster of DAEGrid and ADF bundle with HP-MPI (Amsterdam Density Functional, version 2007 - a FORTRAN program for calculations on atoms and molecules) on 'Aryabhatta' cluster. Now the application of ADF is successfully running through scheduler of 'Aryabhatta' cluster.

F) Installation of SYSTAT Software :

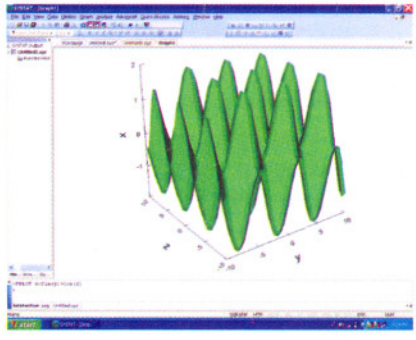

Fig. I.1.2: Graphical plot in SYSTAT-12 software.

Windows based software package SYSTAT (version 12) with five network floating licenses has been installed for users. SYSTAT is a powerful and versatile statistical software package. It provides a menu-driven interface to conduct simple analyses and produce 2D and 3D graphics for engineering and scientific data. Three days training session with hands-on was also organized for SYSTAT users at User Hall, Computer Centre.

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